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FILE LAST UPDATED: 30 Jan 2004  (20040130/ED)

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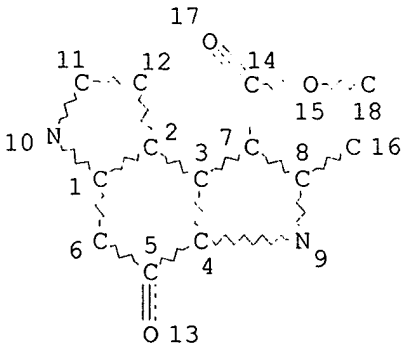


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DEFAULT ECLEVEL IS LIMITED

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NUMBER OF NODES IS  18

STEREO ATTRIBUTES: NONE
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L10               STR
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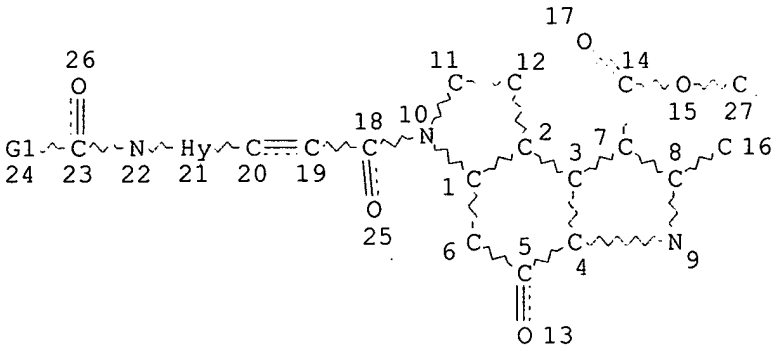

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DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 27

STEREO ATTRIBUTES: NONE
L11 30 SEA FILE=REGISTRY SUB=L9 SSS FUL L10
L12 14 SEA FILE=HCAPLUS ABB=ON PLU=ON L11

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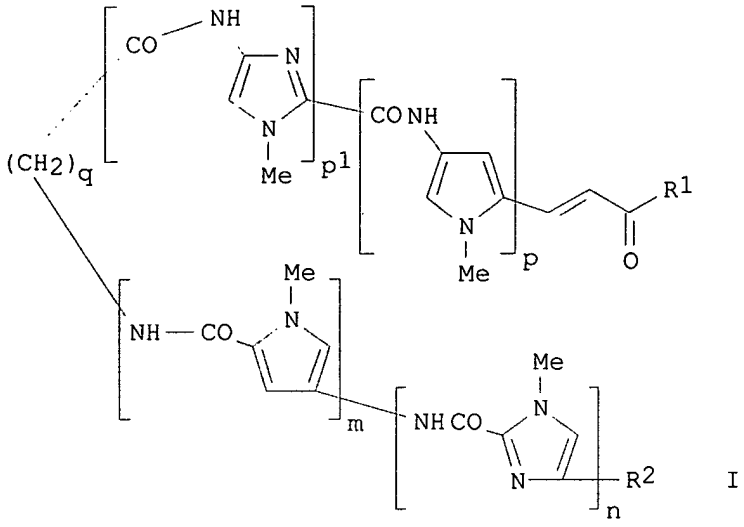
=>

=> d ibib abs hitrn l12 1-14

L12 ANSWER 1 OF 14 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:737733 HCAPLUS
DOCUMENT NUMBER: 139:276894
TITLE: Preparation of hairpin-type pyrrole-imidazole polyamides as anticancer agents
INVENTOR(S): Sugiyama, Hiroshi; Bando, Toshikazu; Saito, Isao
PATENT ASSIGNEE(S): Japan Science and Technology Corporation, Japan
SOURCE: PCT Int. Appl., 46 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003076412	A1	20030918	WO 2003-JP2423	20030303
W: US				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR				
JP 2003261541	A2	20030919	JP 2002-63608	20020308

PRIORITY APPLN. INFO.: JP 2002-63608 A 20020308
OTHER SOURCE(S): MARPAT 139:276894
GI



I

AB It is intended to provide a pyrrole-imidazole polyamide type functional mol. having enhanced abilities of alkylating DNA and recognizing a sequence, compared with the existing functional mols. of this type, for a specific base sequence occurring on DNA. Hairpin polyamides have an alkylation site via a vinyl linker at the end of a pyrrole-imidazole polyamide and are represented by general formula (I; R1 = a site for alkylation reaction; R2 = H, alkyl, acetamido; p, p1, q, m, n = an integer). Disclosed are drugs for inhibiting the expression of a specific gene and anticancer agents contg. the above hairpin polyamide. For example, I (m = p = p1 = 1, n = 2, q = 3, R1 = q) selectively alkylated A of the GTCA sequence of DNA (pUC-I'). The compds. I were tested for inhibiting the proliferation of various cancer cells.

IT **491647-63-3P 491647-64-4P 602308-98-5P 602308-99-6P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of hairpin-type pyrrole-imidazole polyamides for alkylating DNA and inhibiting gene expression as anticancer agents)

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 2 OF 14 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:393696 HCAPLUS
DOCUMENT NUMBER: 139:358146
TITLE: Specific alkylation of human telomere repeats by hairpin pyrrole-imidazole polyamide
AUTHOR(S): Takahashi, Ryoko; Bando, Toshikazu; Sugiyama, Hiroshi
CORPORATE SOURCE: Institute of Biomaterials and Bioengineering, Division of Biofunctional Molecules, Tokyo Medical and Dental University, 2-3-10 Surugadai, Kanda, Chiyoda, Tokyo, 101-0062, Japan
SOURCE: Bioorganic & Medicinal Chemistry (2003), 11(12), 2503-2509
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A novel hairpin polyamide-cyclopropapyrroloindole (CPI) conjugate PyImImIm-.gamma.-PyPyPyLDu86 (conjugate 11), which targets human telomere

repeats d(TTAGGG)n/d(CCCTAA)n, was synthesized. High resoln. denaturing PAGE using 44 bp DNA fragments and HPLC product anal. of a synthetic nonanucleotide demonstrated that conjugate 11 alkylates the target adenine in the telomere repeats, 5'-CCCTAA-3'. Examn. of the antitumor activity of conjugate 11 using a panel of 39 cancer cell lines demonstrated that the av. concn. of conjugate 11 required for 50% growth inhibition was 5.75 .mu.M, which is superior to pepleomycin and bleomycin and comparable to cisplatin.

IT **619212-51-0P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(specific alkylation of human telomere repeats by hairpin pyrrole-imidazole polyamide conjugate in cancer cell lines)

REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 3 OF 14 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:341959 HCAPLUS
DOCUMENT NUMBER: 139:345455
TITLE: Gene therapy of cancer by using novel alkylating pyrrole-imidazole polyamide
AUTHOR(S): Sugiyama, Hiroshi
CORPORATE SOURCE: Dep. of Biomaterials, Tokyo Medical and Dental University, Japan
SOURCE: Ikagaku Oyo Kenkyu Zaidan Kenkyu Hokoku (2001), Volume Date 2000, 19, 198-202
CODEN: IOKHEP; ISSN: 0914-5117
PUBLISHER: Ikagaku Oyo Kenkyu Zaidan
DOCUMENT TYPE: Journal
LANGUAGE: Japanese

AB Novel alkylating pyrrole-imidazole polyamide derivs. were design and prepd. for gene therapy of cancer. The antitumor activities of the derivs. against Hela cells were tested.

IT **339984-88-2P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(gene therapy of cancer by using novel alkylating pyrrole-imidazole polyamides)

IT **339984-91-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(gene therapy of cancer by using novel alkylating pyrrole-imidazole polyamides)

L12 ANSWER 4 OF 14 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:155388 HCAPLUS
DOCUMENT NUMBER: 138:333279
TITLE: Highly Efficient Sequence-Specific DNA Interstrand Cross-Linking by Pyrrole/Imidazole CPI Conjugates
AUTHOR(S): Bando, Toshikazu; Narita, Akihiko; Saito, Isao; Sugiyama, Hiroshi
CORPORATE SOURCE: Division of Biofunctional Molecules Institute of Biomaterials and Bioengineering, Tokyo Medical and Dental University, Tokyo, 101-0062, Japan
SOURCE: Journal of the American Chemical Society (2003), 125(12), 3471-3485
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:333279

AB We have developed a novel type of DNA interstrand crosslinking agent by synthesizing dimers of a pyrrole (Py)/imidazole (Im)-diamide-CPI conjugate, ImPyLDu86, connected using seven different linkers. The tetramethylene linker compd. [I], efficiently produces DNA interstrand-cross-links at the nine-base-pair sequence, 5'-PyGGC(T/A)GCCPu-3', only in the presence of a partner triamide, ImImPy. For efficient crosslinking by I with ImImPy, one A.cntdot.T base pair between two recognition sites was required to accommodate the linker region. Elimination of the A.cntdot.T base pair and insertion of an addnl. A.cntdot.T base pair and substitution with a G.cntdot.C base pair significantly reduced the degree of crosslinking. The sequence specificity of the interstrand crosslinking by I was also examd. in the presence of various triamides. The presence of ImImIm slightly reduced the formation of a cross-linked product compared to ImImPy. The mismatch partners, ImPyPy and PyImPy, did not produce an interstrand cross-link product with I, whereas ImPyPy and PyImPy induced efficient alkylation at their matching site with I. The interstrand crosslinking abilities of I were further examd. using denaturing PAGE with 5'-Texas Red-labeled 400- and 67-bp DNA fragments. The sequencing gel anal. of the 400-bp DNA fragment with ImImPy demonstrated that I alkylates several sites on the top and bottom strands, including one interstrand crosslinking match site, 5'-PyGGC(T/A)GCCPu-3'. To obtain direct evidence of interstrand cross-linkages on longer DNA fragments, a simple method using biotin-labeled complementary strands was developed, which produced a band corresponding to the interstrand cross-linked site on both top and bottom strands. Densitometric anal. indicated that the contribution of the interstrand cross-link in the obsd. alkylation bands was approx. 40%. This compd. efficiently cross-linked both strands at the target sequence. The present system consisted of a 1:2 complex of the alkylating agent and its partner ImImPy and caused an interstrand crosslinking in a sequence-specific fashion according to the base-pair recognition rule of Py-Im polyamides.

IT **373362-22-2P 373362-24-4P 373362-26-6P**
373362-27-7P 515867-58-0P 515867-60-4P
515867-62-6P
RL: BSU (Biological study, unclassified); BUU (Biological use, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(crosslinking; sequence-specific DNA interstrand crosslinking by pyrrole/imidazole CPI conjugates)

REFERENCE COUNT: 76 THERE ARE 76 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 5 OF 14 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:954878 HCAPLUS
DOCUMENT NUMBER: 139:30289
TITLE: Regulation of gene expression by sequence-specific alkylating polyamide
AUTHOR(S): Oyoshi, Takanori; Kawakami, Wakana; Bando, Toshikazu; Narita, Akihiko; Sugiyama, Hiroshi
CORPORATE SOURCE: Division of Biofunctional Molecules, Institute of Biomaterials and Bioengineering, Tokyo Medical and Dental University, Tokyo, 101-0062, Japan
SOURCE: Nucleic Acids Research Supplement (2002), 2(Twenty-ninth Symposium on Nucleic Acids Chemistry), 259-260
CODEN: NARSCE
PUBLISHER: Oxford University Press
DOCUMENT TYPE: Journal
LANGUAGE: English

AB In order to investigate the inhibition of gene expression by a new type of hairpin polyamide-CPI conjugate 1, its ability to inhibit transcription in cell free system was investigated. Sequence-selective alkylation of

double-stranded DNA by 1 was investigated by denaturing gel electrophoresis using 1000 bp DNA fragment which codes for green fluorescence protein (GFP) under the control of T7 promoter. Anal. of DNA sequence indicated that 1 alkylated predominantly at the site of 5'-AGTCA-3' in coding region of GFP. The transcript by T7 RNA polymerase using the alkylated DNA as a template was analyzed by PAGE. The results clearly indicate that 1 inhibits transcription by alkylation of coding region at a nanomolar concn.

IT **491647-63-3**
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(regulation of gene expression by sequence-specific alkylating polyamide)

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 6 OF 14 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:840303 HCAPLUS
DOCUMENT NUMBER: 138:132742
TITLE: Molecular design of a pyrrole - imidazole hairpin polyamides for effective DNA alkylation
AUTHOR(S): Bando, Toshikazu; Narita, Akihiko; Saito, Isao; Sugiyama, Hiroshi
CORPORATE SOURCE: Division of Biofunctional Molecules Institute of Biomaterials and Bioengineering, Tokyo Medical and Dental University, Tokyo, 101-0062, Japan
SOURCE: Chemistry--A European Journal (2002), 8(20), 4781-4790
CODEN: CEUJED; ISSN: 0947-6539
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:132742

AB New hairpin polyamide-CPI (CPI = cyclopropylpyrroloindole) conjugates, compds. 12-14, were synthesized and their DNA-alkylating activities compared with the previously prepd. hairpin polyamide, compd. 1, by high-resoln. denaturing gel electrophoresis with 450 base pair (bp) DNA fragments and by HPLC product anal. of the synthetic decanucleotide. In accord with our previous results, alkylation by compd. 1 occurred predominantly at the G moiety of the sequence 5'-AGTCAG-3' (site 3). However, compd. 12, in which the structure of the alkylating moiety of compd. 1 is replaced with segment A of duocarmycin A DU-86 (CPI), did not show any DNA alkylating activity. In clear contrast, the hairpin CPI conjugate 13, which differs from compd. 1 in that it lacks one Py unit and possesses a vinyl linker, alkylated the A of 5'-AGTCAG-3' (site 3) efficiently at nanomolar concns. Alkylation by compd. 14, which has a vinyl linker, occurred at the A of 5'-AGTCCA-3' (site 6) and at several minor alkylation sites, including mismatch alkylation at A of 5'-TCACAA-3' (site 2). The significantly different reactivity of the alkylating hairpin polyamides 1, 12, 13, and 14 was further confirmed by HPLC product anal. by using a synthetic decanucleotide. The results suggest that hairpin polyamide-CPI conjugate 13 alkylates effectively according to Dervan's pairing rule, and with a new mode of recognition in which the Im-vinyl linker (L) pair targets G-C base pairs. These results demonstrate that incorporation of the vinyl-linker pairing with Im dramatically improves the reactivity of hairpin polyamide-CPI conjugates.

IT **491647-63-3P 491647-64-4P**
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(vinyl-linker pairing with imidazole in pyrrole - imidazole hairpin can improve polyamides for effective DNA alkylation)

REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 7 OF 14 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:666652 HCAPLUS
DOCUMENT NUMBER: 138:85083
TITLE: Sequence-specific protection of plasmid DNA from restriction endonuclease hydrolysis by pyrrole-imidazole-cyclopropapyrroloindole conjugates
AUTHOR(S): Fujimoto, Kazuhisa; Iida, Hirokazu; Kawakami, Masako; Bando, Toshikazu; Tao, Zhi-Fu; Sugiyama, Hiroshi
CORPORATE SOURCE: Institute of Biomaterials and Bioengineering, Division of Biofunctional Molecules, Tokyo Medical and Dental University, Chiyoda, Tokyo, 101-0062, Japan
SOURCE: Nucleic Acids Research (2002), 30(17), 3748-3753 - CODEN: NARHAD; ISSN: 0305-1048
PUBLISHER: Oxford University Press
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The pyrrole-imidazole (Py-Im) triamide-cyclopropa pyrroloindole (CPI) conjugates ImPyImLDu86 (7) and ImImPyLDu86 (14) were synthesized and their alkylating activities and inhibitory effects on DNA hydrolysis by restriction endonucleases were examd. Sequencing gel anal. demonstrated that conjugates 7 and 14 specifically alkylated DNA at 5'-CGCGCG-3' and 5'-PyGGCCPu-3', resp. Agarose gel electrophoresis indicated that incubation of a supercoiled plasmid, pSPORT I (4109 bp), with conjugate 7 effectively inhibited its hydrolysis by BssHII (5'-GCGCGC-3'), whereas conjugate 14 had no effect on this hydrolysis. These results suggest that conjugate 7 sequence-specifically inhibits the hydrolysis of DNA by BssHII. Sequence-specific alkylation by the Py-Im triamide-CPI conjugates was further confirmed by inhibition of the Eco52I (5'-CGGCCG-3') hydrolysis of conjugate 14-treated pQBI PGK (5387 bp). In clear contrast, hydrolysis of pQB1 PGK by DraI (3'-TTTAAA-3') was not inhibited by 5 .mu.M conjugate 14. That ImImPy did not inhibit the hydrolysis of pQB1 PGK indicates that covalent bond formation is necessary for inhibition. A similar expt., using linear pQBI PGK, achieved the same extent of protection of the DNA with approx. half the concn. of conjugate 14 as was required to protect supercoiled DNA from hydrolysis.

IT **484017-85-8P 484017-86-9P**
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(sequence-specific protection of plasmid DNA from restriction endonuclease hydrolysis by pyrrole-imidazole-cyclopropapyrroloindole conjugates)

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 8 OF 14 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:833321 HCAPLUS
DOCUMENT NUMBER: 135:371743
TITLE: Preparation of pyrrole-imidazole polyamide-duocarmycin segment conjugates as interstrand crosslinking agents for DNA in cancer treatment
INVENTOR(S): Sugiyama, Hiroshi; Bando, Toshikazu; Iida, Hirokazu; Saito, Isao
PATENT ASSIGNEE(S): Japan Science and Technology Corporation, Japan
SOURCE: PCT Int. Appl., 54 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001085733	A1	20011115	WO 2001-JP3756	20010501

W: US
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR

JP 2001322992	A2	20011120	JP 2000-140361	20000512
EP 1281711	A1	20030205	EP 2001-926081	20010501

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY, TR

PRIORITY APPLN. INFO.: JP 2000-140361 A 20000512
WO 2001-JP3756 W 20010501

OTHER SOURCE(S): MARPAT 135:371743
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Compds. represented by the following general formula A-L-B-X-B-L-A (I; wherein B represents a chem. structure capable of recognizing a base sequence of a DNA; A represents a chem. structure capable of binding to one of the bases of the DNA; L represents a linker by which the chem. structures A and B can be linked to each other; and X represents a spacer by which the A-L-B components can be linked to each other), by which two DNA strands can be interstrand-crosslinked, are prepd. Also claimed are a method of interstrand-crosslinking DNA by using these compds. and medicinal compns. contg. interstrand crosslinking agents of DNA. In the compds. I, the above chem. structure capable of recognizing a base sequence of a DNA is derived from pyrrole and/or imidazole and the chem. structure capable of binding to one of the bases of the DNA possesses a cyclopropane ring. More specifically, the compds. represented by N-[3-[4-(N-methylimidazol-2-ylcarbonylamino)-N-methylpyrrol-2-yl]acryloyl]cyclopropa[c]pyrrolo[3,2-e]indole derivs. (pyrrole-imidazole polyamide-duocarmycin segment conjugates) [II; X = CO, COCH:CHCO, CO(CH2)4CO, CO-p-C6H4-CO] are prepd. The B component in the compds. I, i.e. the 4-(N-methylimidazol-2-ylcarbonylamino)-N-methylpyrrole moiety of II, recognizes a DNA base sequence and is capable of specifically interstrand-crosslinking to the specific base sequence of DNA. These compds. inhibit the replication of DNA by interstrand-crosslinking to DNA and thereby are useful for the treatment of cancer. Interstrand-crosslinking reaction of the compds. II to DNA oligomers was examd. using polyacrylamide gel electrophoresis. For example, it was confirmed that II [X = CO(CH2)4CO] interstrand-crosslinked to the TGGC or GCCA or its complimentary sequence of DNA, in particular in the copresence of a triamide (III; X = Y = N and Z = CH; X = Y = Z = N; X = N and Y = Z = CH; X = Z = CH and Y = N).

IT **373362-22-2P 373362-24-4P 373362-26-6P**
373362-27-7P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of pyrrole-imidazole polyamide-duocarmycin conjugates as DNA interstrand crosslinking agents for treatment of cancer)

REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 9 OF 14 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:365880 HCAPLUS
DOCUMENT NUMBER: 134:366795
TITLE: DNA sequence recognition by pyrrole-imidazole polyamide for use in anticancer drug screening
INVENTOR(S): Sugiyama, Hiroshi; Saito, Akira; Iida, Hirokazu
PATENT ASSIGNEE(S): Foundation for Scientific Technology Promotion, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 14 pp.

CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2001136974	A2	20010522	JP 1999-326007	19991116
WO 2001036677	A1	20010525	WO 2000-JP7992	20001113
W: US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
EP 1152061	A1	20011107	EP 2000-974961	20001113
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
US 2003099998	A1	20030529	US 2002-285030	20021101

PRIORITY APPLN. INFO.: JP 1999-326007 A 19991116
WO 2000-JP7992 W 20001113
US 2001-889379 A3 20010716

AB Novel chem. species represented by the following general formula B-L-A (B = a chem. structure capable of recognizing the base sequence of DNA, for example, optionally substituted pyrrole-imidazole polyamide; A = a chem. structure capable of binding to unnatural nucleotide bases, for example, the alkylation moiety of duocarmycin A; L = a linker capable of binding the chem. structures A and B, for example, vinyl) and use of those compds. in screening of biol. activity of chem. compds. are disclosed. Those compds. are preferably DNA alkylating agents, applicable as anticancer agents. Reagent kits for screening, including microtiter plates, are claimed. Drug screening using human cancer cell lines, CL-wt cells, HLC-2 cells, Jurkat cells, and HeLa cells, and synthetic scheme for the bioactive compds., are described.

IT **339984-88-2 339984-91-7**
RL: ARU (Analytical role, unclassified); BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); BUU (Biological use, unclassified); PRP (Properties); ANST (Analytical study); BIOL (Biological study); PROC (Process); USES (Uses)
(DNA sequence recognition by pyrrole-imidazole polyamide for use in anticancer drug screening)

IT **339984-92-8P**
RL: ARU (Analytical role, unclassified); BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); BUU (Biological use, unclassified); PRP (Properties); SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
(DNA sequence recognition by pyrrole-imidazole polyamide for use in anticancer drug screening)

L12 ANSWER 10 OF 14 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:327062 HCAPLUS
DOCUMENT NUMBER: 135:102536
TITLE: Sequence-specific DNA interstrand cross-linking by imidazole-pyrrole CPI conjugate
AUTHOR(S): Bando, Toshikazu; Iida, Hirokazu; Saito, Isao; Sugiyama, Hiroshi
CORPORATE SOURCE: CREST Japan Science and Technology Corporation (JST) Japan Division of Biofunctional Molecules Institute of Biomaterials and Bioengineering Tokyo Medical and Dental University, Kanda Chiyoda Tokyo, 101-0062, Japan
SOURCE: Journal of the American Chemical Society (2001), 123(21), 5158-5159

CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB DNA interstrand crosslinking inhibits both DNA replication and gene expression and therefore has considerable potential for mol. biol. and human medicine. However, an interstrand crosslinking agent that targets a predetd. base-pair sequence has not been achieved. Minor-groove binding polyamides that contain N-methylimidazole (Im)-N-methylpyrrole (Py)hydroxypyrrole (Hp), which uniquely recognize each of the four Watson-Crick base pairs, can be used as novel recognition parts of sequence-specific DNA alkylating agents. We also demonstrated that Im/Py diamide-CPI conjugate with a vinyl linker, ImPyLDu86, alkylates double-stranded DNA at predetd. sequences through highly cooperative homodimer formation. Herein we describe the synthesis of a covalent dimer of ImPyLDu86 connected with various linkers and their DNA interstrand crosslinking abilities. In conclusion, we developed a novel DNA interstrand crosslinking agent, that crosslinked double strands only in the presence of ImImPy at a nine-base-pair sequence, 5'-PyGGC(T/A)GCCPu-3'. The present system will provide a promising approach for the design of novel sequence-specific DNA interstrand crosslinking agents. Targeting specific sequences in the human genome by such sequence-specific crosslinking agent would constitute a powerful gene-regulating tool. Further studies on the applicability of this novel class of crosslinking agents are currently in progress.

IT **349647-78-5 349647-79-6 349647-80-9**
349647-82-1 349647-83-2
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(sequence-specific DNA interstrand crosslinking by imidazole-pyrrole CPI conjugate)

IT **349647-81-0P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(sequence-specific DNA interstrand crosslinking by imidazole-pyrrole CPI conjugate)

REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 11 OF 14 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2000:707167 HCAPLUS
DOCUMENT NUMBER: 133:266852
TITLE: Preparation of duocarmycin derivatives capable of cleaving double-stranded DNA and method of utilization of the same
INVENTOR(S): Sugiyama, Hiroshi; Tao, Zhi-Fu; Saito, Isao
PATENT ASSIGNEE(S): Japan Science and Technology Corporation, Japan
SOURCE: PCT Int. Appl., 28 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000058312	A1	20001005	WO 2000-JP1461	20000310
W: CA, KR, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
JP 2000281679	A2	20001010	JP 1999-83591	19990326
CA 2328903	AA	20001005	CA 2000-2328903	20000310

EP 1083177 A1 20010314 EP 2000-907992 20000310
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI
PRIORITY APPLN. INFO.: JP 1999-83591 A 19990326
WO 2000-JP1461 W 20000310

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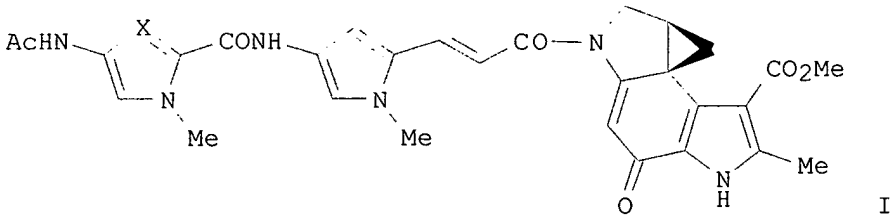


I

AB Novel chem. species represented by the following general formula B-L-A (I; wherein B represents a chem. structure capable of recognizing the base sequence of DNA, for example, optionally substituted pyrrole-imidazole polyamide; A represents a chem. structure capable of binding to one base of DNA, for example, the alkylation moiety of duocarmycin A; and L represents a linker capable of binding the chem. structures A and B, for example, vinyl) are prepd. Also claimed are a method for alkylating DNA and a method for cleaving double-stranded DNA by using these compds.; and medicinal compns. with the use of these compds. for treatment of cancer. These compds. I, e.g. duocarmycin derivs. (II; R = CH, N) (prepn. given) which recognizes base sequences TGACG or CGACG or their complimentary chain, are capable of simultaneously alkylating double-stranded DNA and cleaving the same and useful as artificial restriction enzymes or for targeting specific DNA base sequences for gene therapy. II (R = CH), II (R = N), and duocarmycin A in vitro showed IC50 of 1.5, 0.7 nM, and 4.7, resp., for inhibiting the proliferation of HeLaS3 cells.

IT **296794-37-1P 296794-38-2P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of duocarmycin derivs. capable of alkylating and cleaving double-stranded DNA as anticancer agents)

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 12 OF 14 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2000:96276 HCAPLUS
DOCUMENT NUMBER: 132:275556
TITLE: Highly cooperative DNA dialkylation by the homodimer of imidazole-pyrrole diamide-CPI conjugate with vinyl linker
AUTHOR(S): Tao, Zhi-Fu; Saito, Isao; Sugiyama, Hiroshi
CORPORATE SOURCE: CREST, Japan Science and Technology Corporation (JST), Japan
SOURCE: Journal of the American Chemical Society (2000), 122(8), 1602-1608
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 132:275556

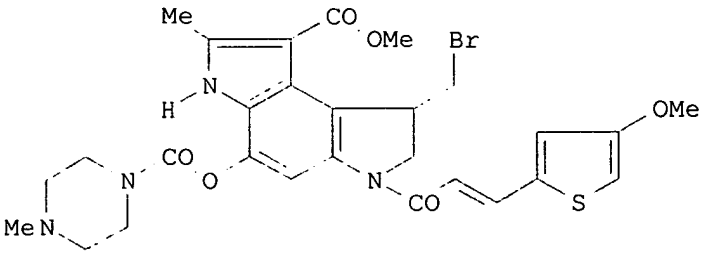
AB We synthesized new type of diamide-CPI conjugate possessing a vinyl linker (7). Sequence-selective alkylation of double-stranded DNA by 7 was investigated by high-resoln. denaturing gel electrophoresis using

.apprx.400 bp DNA fragments. Highly efficient alkylation predominantly occurs simultaneously at the purines of 5'-PyG(A/T)CPu-3' site on both strands at a nanomolar concn. of 7. These results suggest that the homodimer of conjugate 7 dialkylates both strands according to Dervan's pairing rule together with a new mode of recognition in which the Im-vinyl linker (L) pair targets G/C base pairs. In addn. to the major dialkylation sites, a minor alkylation site was also obsd. at 5'-GT(A/T)GC-3'. This alkylation can be explained by an analogous slipped homodimer recognition mode in which the L-L pair recognizes the A/T base pair. Efficient dialkylation by the homodimer of 7 was further confirmed using oligonucleotides (ODNs). HPLC anal. revealed that the conjugate 7 simultaneously alkylates GN3/AN3 of the target sequences on both strands of ODNs.

IT **263710-69-6P**
RL: NUU (Other use, unclassified); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(prepn. and cooperative DNA dialkylation by imidazole-pyrrole diamide-CPI conjugate with vinyl linker)

REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 13 OF 14 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:674932 HCAPLUS
DOCUMENT NUMBER: 132:22791
TITLE: Synthesis and antitumor activity of duocarmycin derivatives: a-ring pyrrole compounds bearing 5-membered heteroarylacryloyl groups
AUTHOR(S): Amishiro, Nobuyoshi; Nagamura, Satoru; Kobayashi, Eiji; Okamoto, Akihiko; Gomi, Katsushige; Saito, Hiromitsu
CORPORATE SOURCE: Pharmaceutical Research Institute, Kyowa Hakko Kogyo Company, Ltd., Shizuoka, 411-8731, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1999), 47(10), 1393-1403
CODEN: CPBTAL; ISSN: 0009-2363
PUBLISHER: Pharmaceutical Society of Japan
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 132:22791
GI



I

AB A series of A-ring pyrrole compds. of duocarmycin bearing 5-membered heteroarylacryloyl groups (thienylacryloyl and pyrrolylacryloyl) and heteroarylcarbonyl groups were synthesized and evaluated for in vitro anticellular activity against HeLa S3 cells and in vivo antitumor activity against murine sarcoma 180 in mice. Most of the thienylacrylates displayed in vitro anticellular activity equiv. to 4'-methoxycinnamates. Among the 8-O-[(N-methylpiperazinyl)carbonyl] derivs. of

methoxy-thienylacrylates, compd. I, having 4'-methoxy-2'-thienylacryloyl as segment-B (Seg-B), showed remarkably potent antitumor activity and low peripheral blood toxicity in vivo, which were equal to those of 8-O-[(N-methylpiperazinyl)carbonyl] derivs. of 4'-methoxycinnamates, compared with the A-ring pyrrole derivs. having the trimethoxyindole skeleton in Seg-B. On the other hand, the 2'-pyrrolylacrylates having a double bond as spacer showed 102- to 103-fold stronger anticellular activity than 2'-pyrrolecarboxylates (IC50<0.3 nM, 72h-exposure). The 8-O-acetate and 8-O-[(N-methylpiperazinyl)carbonyl] derivs. of 2'-pyrrolylacrylates exhibited an antitumor effect at a lower dose compared with the 8-O-[(N-methylpiperazinyl)carbonyl] derivs. with a 4'-methoxycinnamoyl moiety. Moreover, it was expected that the antitumor activity would be increased by the strength of the extra hydrogen bond formed between the nitrogen of the pyrrole amido group and DNA, owing to the increase of the no. of N-methyl-2'-pyrrolecarboxamide units. However, 2'-pyrrolylacrylates having three N-methyl-2'-pyrrolecarboxamide units showed nearly equal antitumor activity to 2'-pyrrolylacrylates having only one N-methyl-2'-pyrrolecarboxamide unit.

IT **251999-80-1P 251999-81-2P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and antitumor activity of duocarmycin derivs. bearing 5-membered heteroarylacryloyl groups)

REFERENCE COUNT: 74 THERE ARE 74 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 14 OF 14 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1998:87732 HCAPLUS
DOCUMENT NUMBER: 128:154100
TITLE: Preparation of DC-89 derivatives as antitumor agents
INVENTOR(S): Amishiro, Nobuyoshi; Saito, Hiromitsu; Okamoto, Akihiko; Gomi, Katsushige; Okabe, Masami
PATENT ASSIGNEE(S): Kyowa Hakko Kogyo Co., Ltd., Japan; Amishiro, Nobuyoshi; Saito, Hiromitsu; Okamoto, Akihiko; Gomi, Katsushige; Okabe, Masami
SOURCE: PCT Int. Appl., 57 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9803509	A1	19980129	WO 1997-JP2516	19970722
W: AU, BG, BR, CA, CN, CZ, HU, JP, KR, MX, NO, NZ, PL, RO, SG, SI, SK, UA, US, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 9734631	A1	19980210	AU 1997-34631	19970722
PRIORITY APPLN. INFO.:			JP 1996-192634	19960723
			WO 1997-JP2516	19970722

OTHER SOURCE(S): MARPAT 128:154100
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. (I) wherein (II) represents (III) or (IV) [X = Cl, Br; R = H, COR1, etc.; R1 = H, (un)substituted alkyl, etc.], and W represents (V) or (VI) (Y1, Y2 = O, S, etc.; Q1-Q5 = H, alkoxy, NO2, etc.; m = 0-1; n

= 0-2), are prepd. I are useful as antitumor agents. Compd. (VII) was treated with NaH and then reacted with compd. (VIII) to give 73% the title compd. (IX), which showed IC50 of 2.9 nM against HeLaS3 cell.

IT **202419-12-3P 202419-15-6P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of DC-89 derivs. as antitumor agents)

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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=> fil caold
FILE 'CAOLD' ENTERED AT 17:56:13 ON 31 JAN 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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FILE COVERS 1907-1966
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

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STRUCTURE FILE UPDATES: 30 JAN 2004 HIGHEST RN 644468-14-4
DICTIONARY FILE UPDATES: 30 JAN 2004 HIGHEST RN 644468-14-4

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

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Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

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=> d ide can l11 tot

L11 ANSWER 1 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN
RN 619212-51-0 REGISTRY
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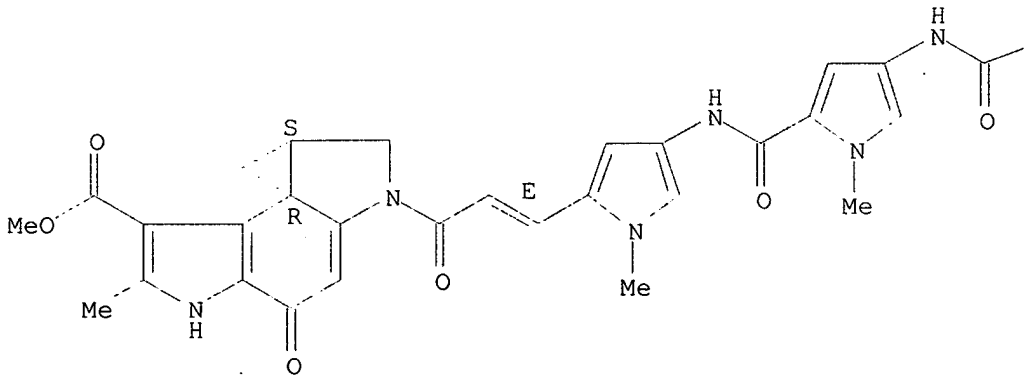
FS STEREOSEARCH
MF C61 H64 N20 O12
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



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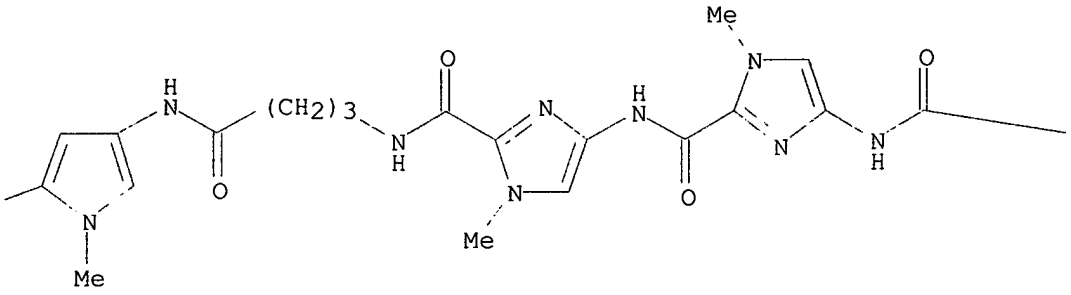

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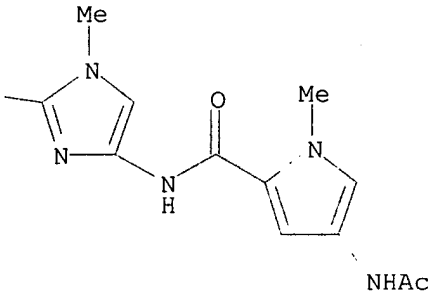

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1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 139:358146

L11 ANSWER 2 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN
RN 602308-99-6 REGISTRY
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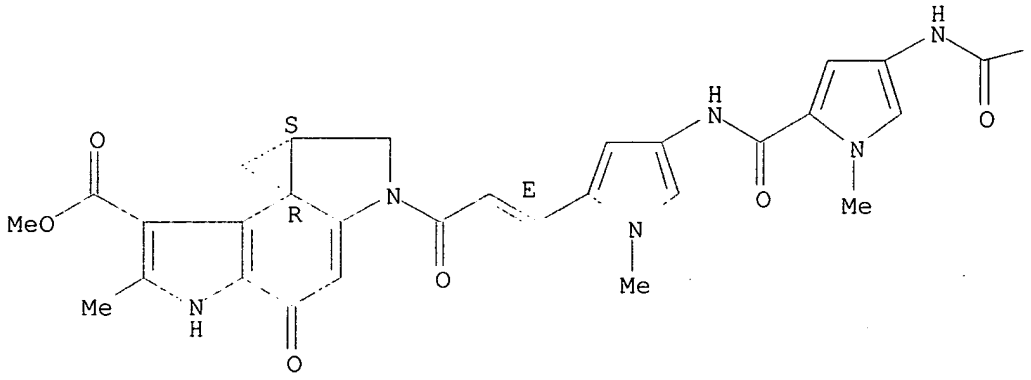
FS STEREOSEARCH
MF C59 H61 N19 O11
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



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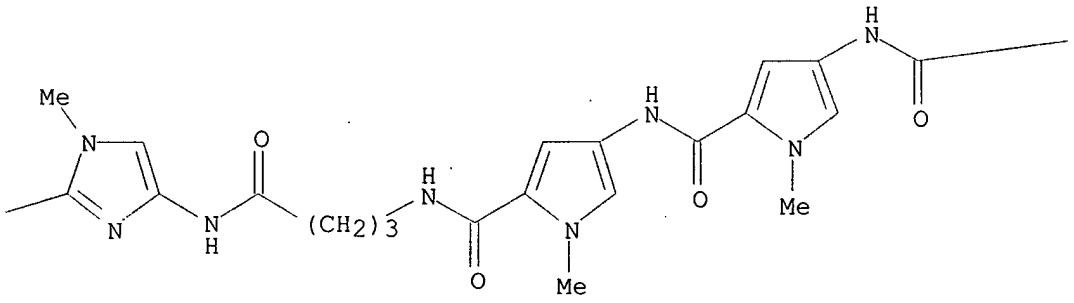

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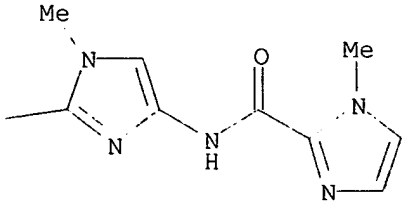

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1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 139:276894

L11 ANSWER 3 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN
RN 602308-98-5 REGISTRY
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FS STEREOSEARCH
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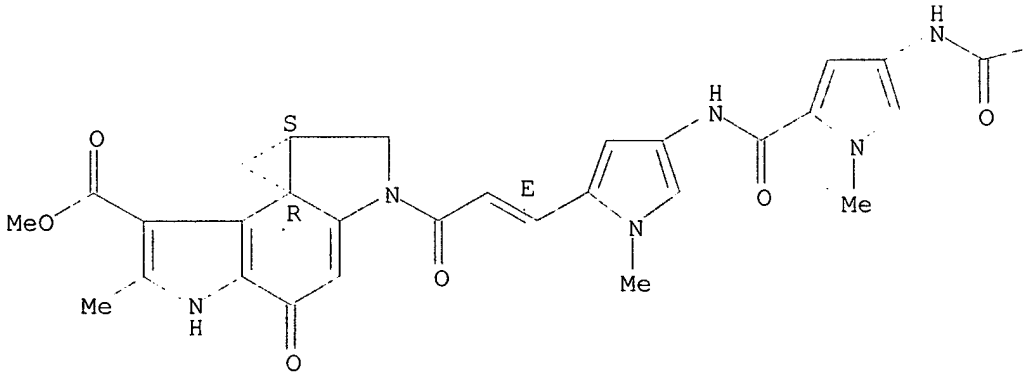
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



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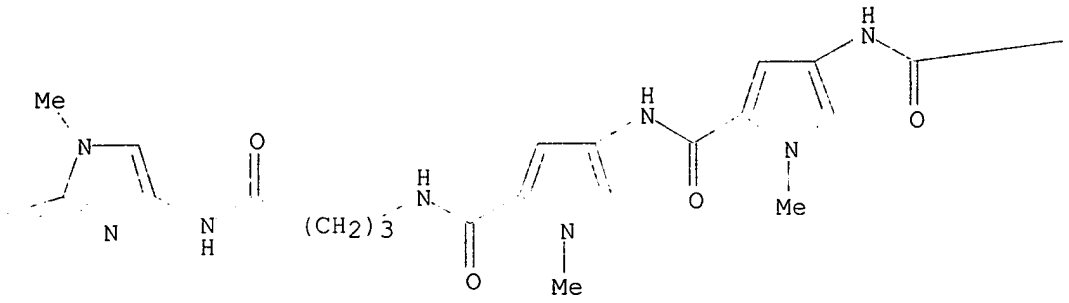

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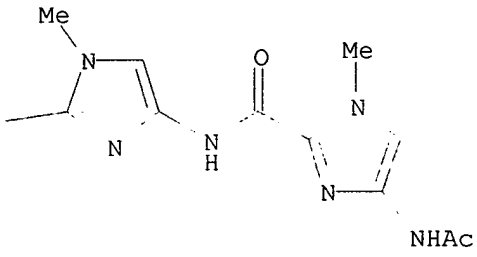

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1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 139:276894

L11 ANSWER 4 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN
RN 515867-62-6 REGISTRY
CN Cyclopropa[c]pyrrolo[3,2-e]indole-7-carboxylic acid, 2,2'-[1,3-phenylenebis[carbonylimino(1-methyl-1H-imidazole-4,2-diyl)carbonylimino(1-methyl-1H-pyrrole-4,2-diyl)[(2E)-1-oxo-2-propene-3,1-diyl]]]bis[1,2,4,5,8,8a-hexahydro-6-methyl-4-oxo-, dimethyl ester, (7bR,7'bR,8aS,8'aS)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
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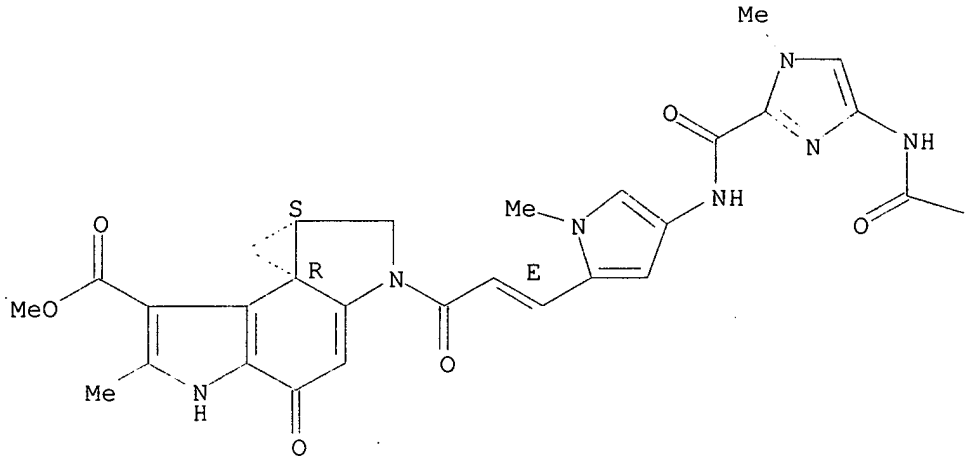
SR CA
LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



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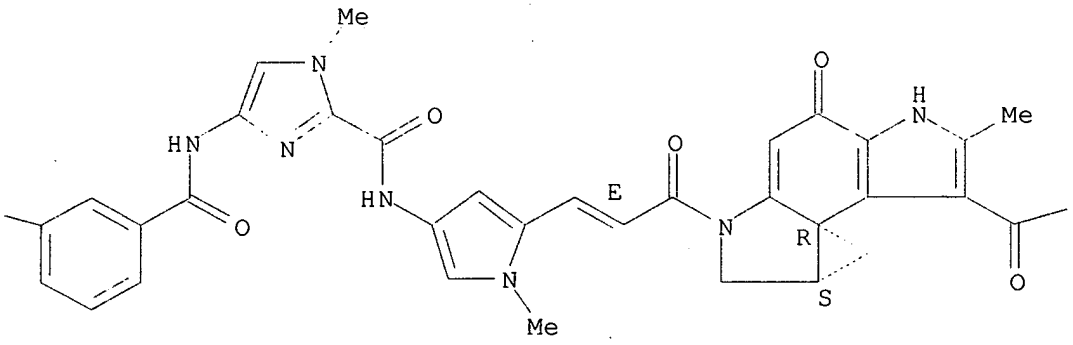

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1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:333279

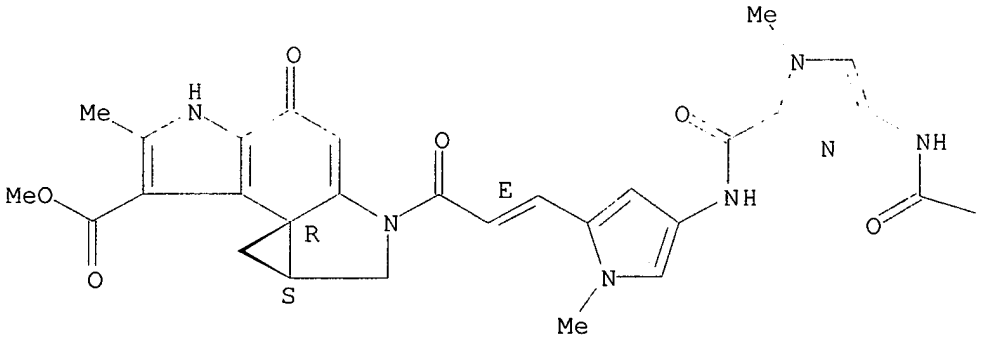
L11 ANSWER 5 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN
RN 515867-60-4 REGISTRY
CN Cyclopropa[c]pyrrolo[3,2-e]indole-7-carboxylic acid, 2,2'-[(1,7-dioxo-1,7-

heptanediyl)bis[imino(1-methyl-1H-imidazole-4,2-diyl)carbonylimino(1-methyl-1H-pyrrole-4,2-diyl)[(2E)-1-oxo-2-propene-3,1-diyl]]]bis[1,2,4,5,8,8a-hexahydro-6-methyl-4-oxo-, dimethyl ester, (7bR,7'bR,8aS,8'aS)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH
MF C61 H62 N14 O12
SR CA
LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



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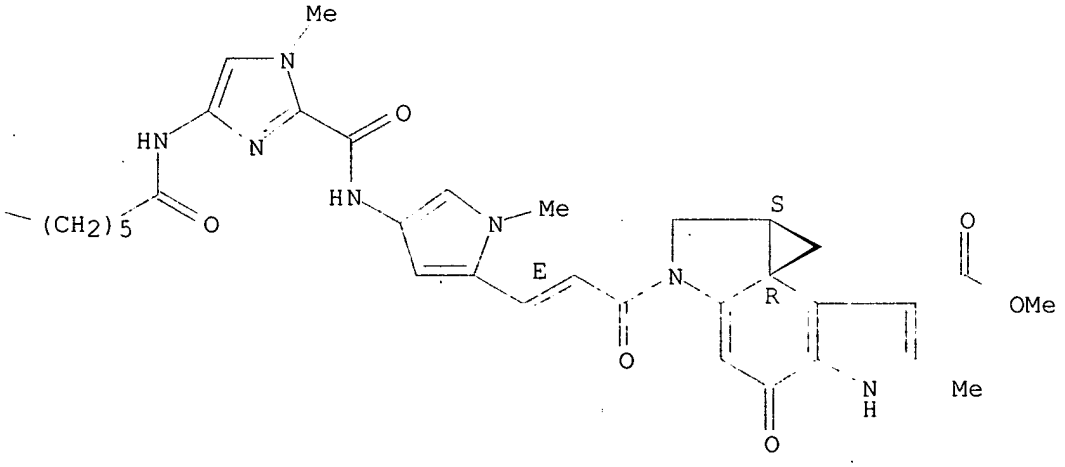

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1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:333279

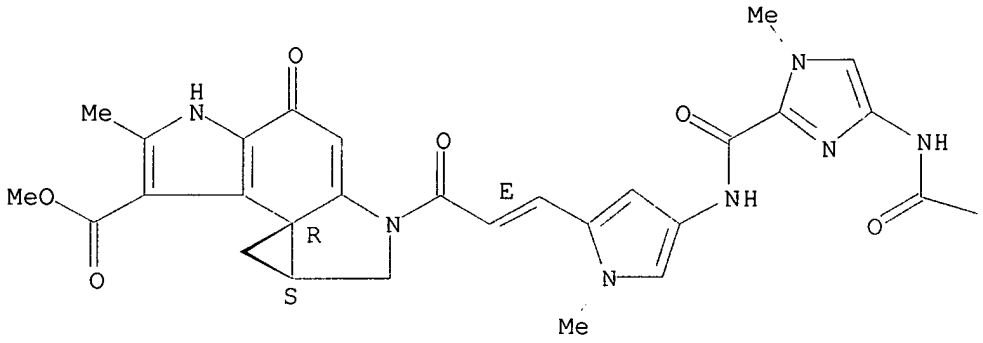
L11 ANSWER 6 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN
RN 515867-58-0 REGISTRY
CN Cyclopropa[c]pyrrolo[3,2-e]indole-7-carboxylic acid, 2,2'-[(1,5-dioxo-1,5-pentanediyl)bis[imino(1-methyl-1H-imidazole-4,2-diyl)carbonylimino(1-

methyl-1H-pyrrole-4,2-diyl]{(2E)-1-oxo-2-propene-3,1-diyl]]]bis[1,2,4,5,8,8a-hexahydro-6-methyl-4-oxo-, dimethyl ester, (7bR,7'bR,8aS,8'aS)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH
MF C59 H58 N14 O12
SR CA
LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



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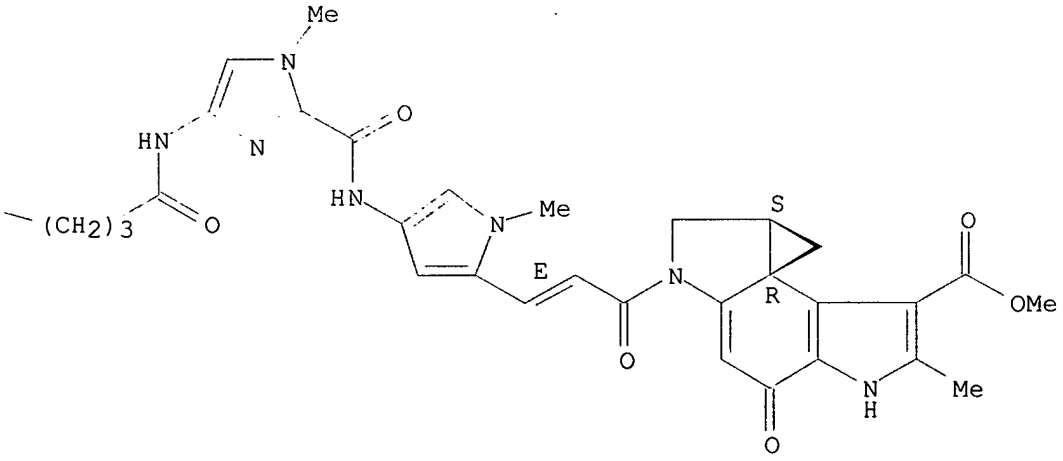


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:333279

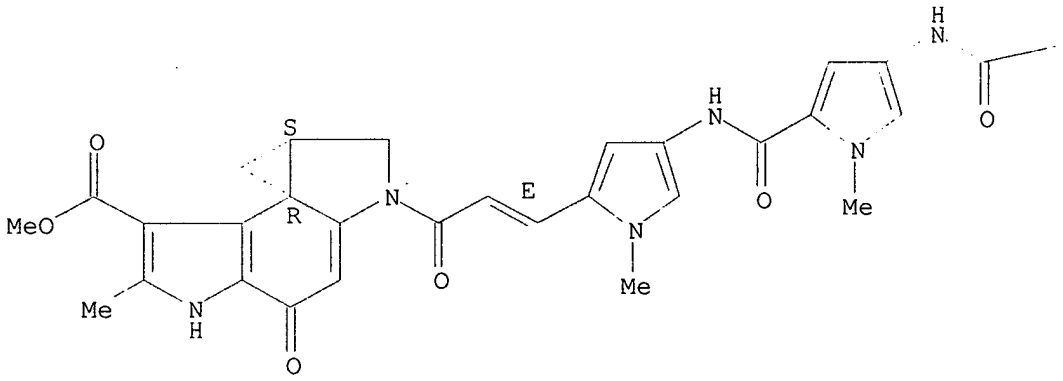
L11 ANSWER 7 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN
RN 491647-64-4 REGISTRY
CN Cyclopropa[c]pyrrolo[3,2-e]indole-7-carboxylic acid, 2-[(2E)-3-[4-[[[4-[[[4-[[4-[[[4-[[[4-[[[4-(acetylamino)-1-methyl-1H-imidazol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-1H-

pyrrol-2-yl]carbonyl]amino]-1-oxobutyl]amino]-1-methyl-1H-imidazol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]-1-oxo-2-propenyl]-1,2,4,5,8,8a-hexahydro-6-methyl-4-oxo-, methyl ester, (7bR,8aS)- (9CI) (CA INDEX NAME)

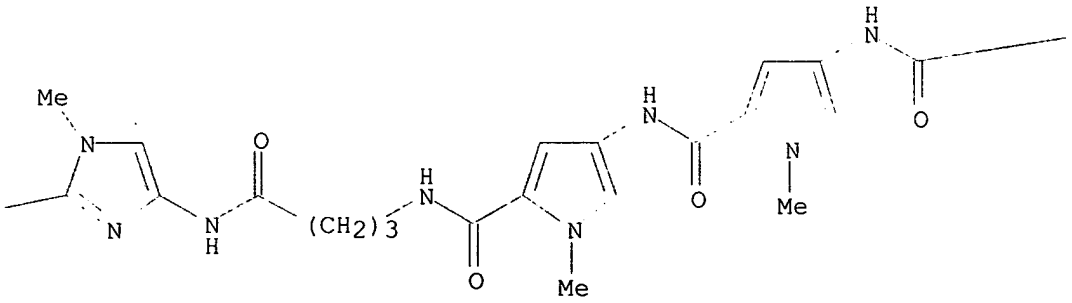
FS STEREOSEARCH
MF C56 H59 N17 O11
SR CA
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



PAGE 1-B



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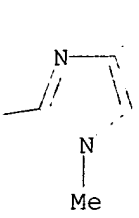


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

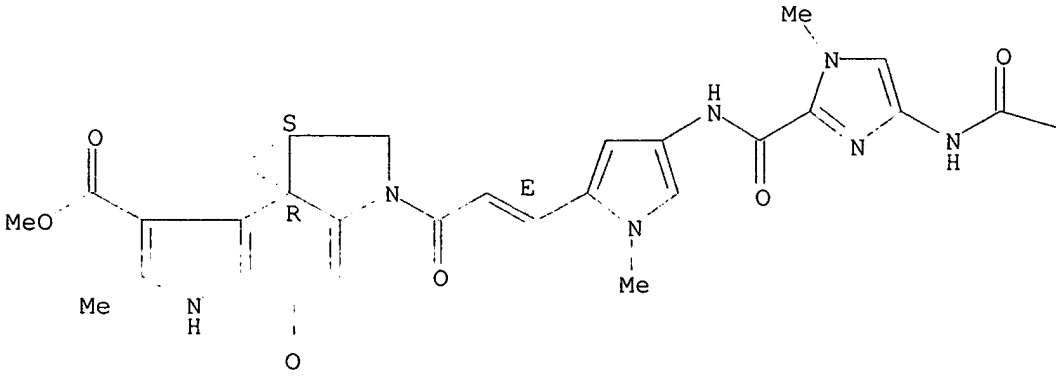
REFERENCE 1: 139:276894

REFERENCE 2: 138:132742

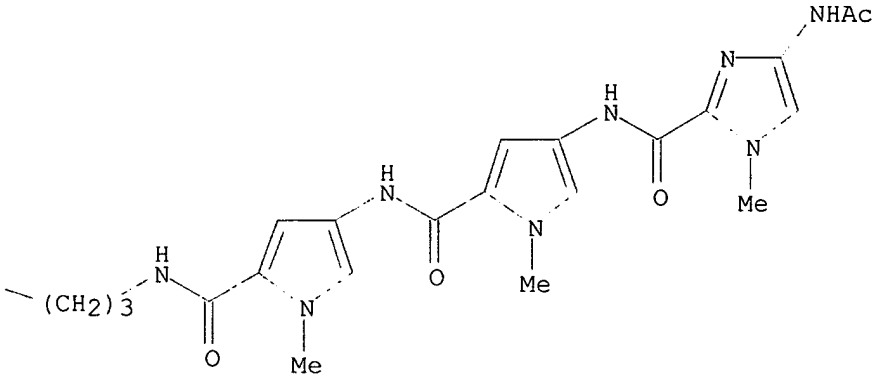
L11 ANSWER 8 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN
RN 491647-63-3 REGISTRY
CN Cyclopropa[c]pyrrolo[3,2-e]indole-7-carboxylic acid, 2-[(2E)-3-[4-[[[4-[[4-[[[4-[[[4-[[[4-(acetylamino)-1-methyl-1H-imidazol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-oxobutyl]amino]-1-methyl-1H-imidazol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]-1-oxo-2-propenyl]-1,2,4,5,8,8a-hexahydro-6-methyl-4-oxo-, methyl ester, (7bR,8aS)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C50 H53 N15 O10
SR CA
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



PAGE 1-B



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 139:276894

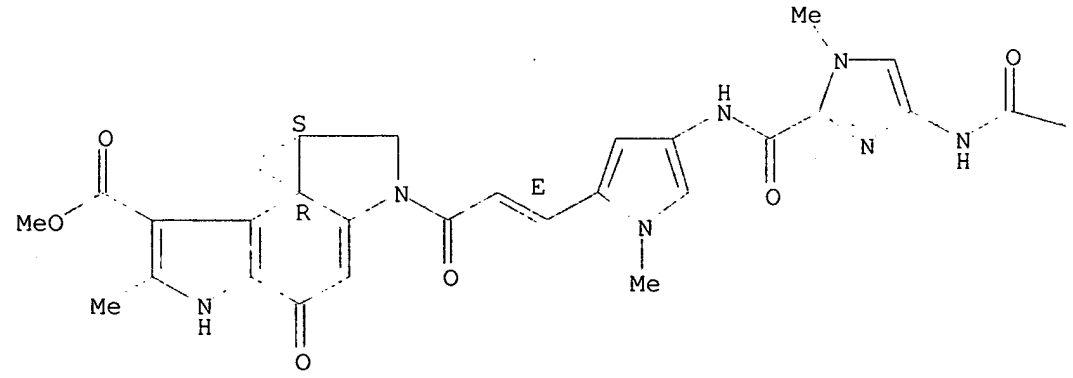
REFERENCE 2: 139:30289

REFERENCE 3: 138:132742

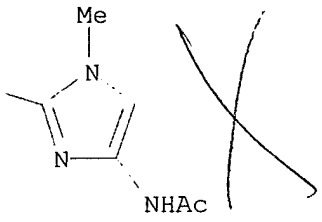
L11 ANSWER 9 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN
RN 484017-86-9 REGISTRY
CN Cyclopropa[c]pyrrolo[3,2-e]indole-7-carboxylic acid, 2-[(2E)-3-[4-[[[4-[[[4-(acetylamino)-1-methyl-1H-imidazol-2-yl]carbonyl]amino]-1-methyl-1H-imidazol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]-1-oxo-2-propenyl]-1,2,4,5,8,8a-hexahydro-6-methyl-4-oxo-, methyl ester, (7bR,8aS)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C34 H34 N10 O7
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



PAGE 1-B



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

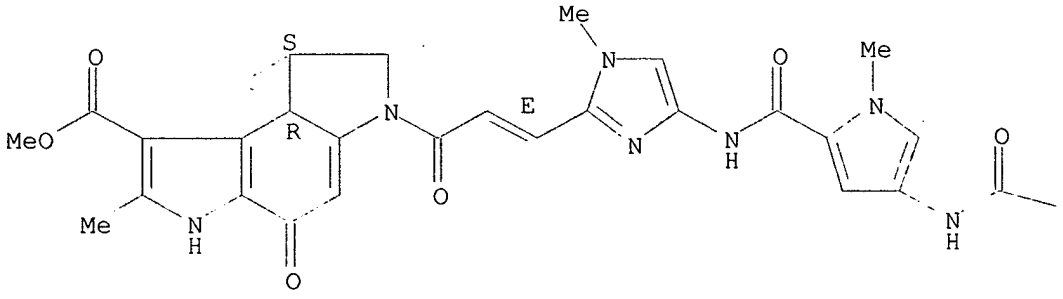
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:85083

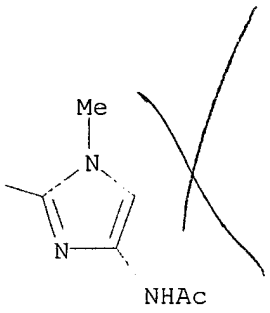
L11 ANSWER 10 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN
RN 484017-85-8 REGISTRY
CN Cyclopropa[c]pyrrolo[3,2-e]indole-7-carboxylic acid, 2-[(2E)-3-[4-[[[4-[[[4-(acetylamino)-1-methyl-1H-imidazol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-1H-imidazol-2-yl]-1-oxo-2-propenyl]-1,2,4,5,8,8a-hexahydro-6-methyl-4-oxo-, methyl ester, (7bR,8aS)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C34 H34 N10 O7
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



PAGE 1-B



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

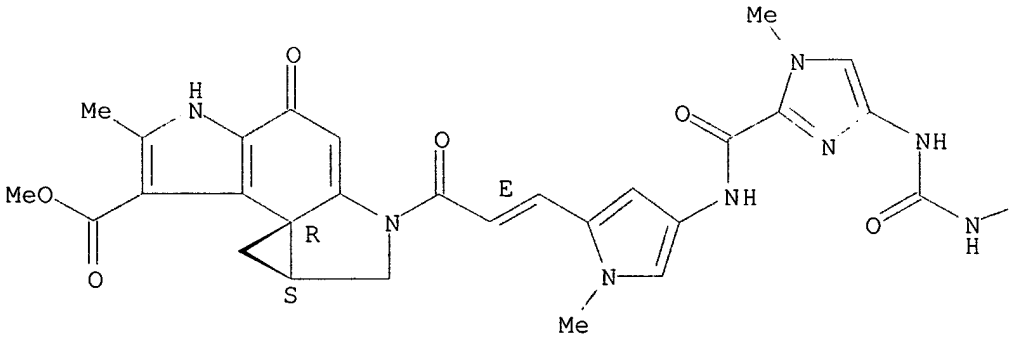
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:85083

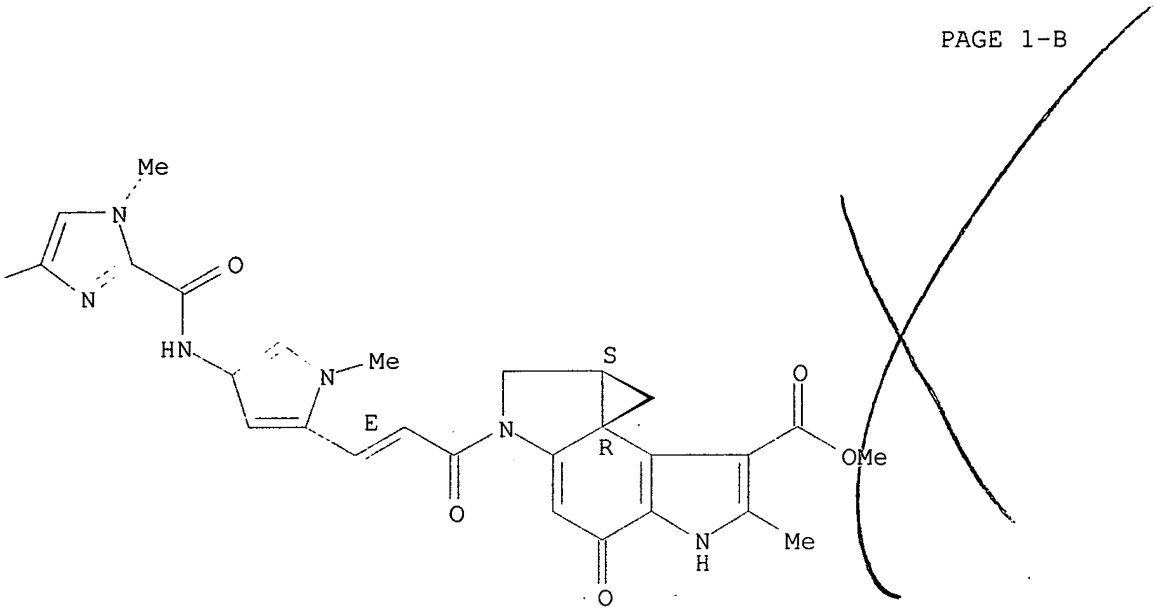
L11 ANSWER 11 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN
RN 373362-27-7 REGISTRY
CN Cyclopropa[c]pyrrolo[3,2-e]indole-7-carboxylic acid, 2,2'-[carbonylbis[imino(1-methyl-1H-imidazole-4,2-diyl)carbonylimino(1-methyl-1H-pyrrole-4,2-diyl)[(2E)-1-oxo-2-propene-3,1-diyl]]]bis[1,2,4,5,8,8a-hexahydro-6-methyl-4-oxo-, dimethyl ester, (7bR,7'bR,8aS,8'aS)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C55 H52 N14 O11
SR CA
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



PAGE 1-B



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

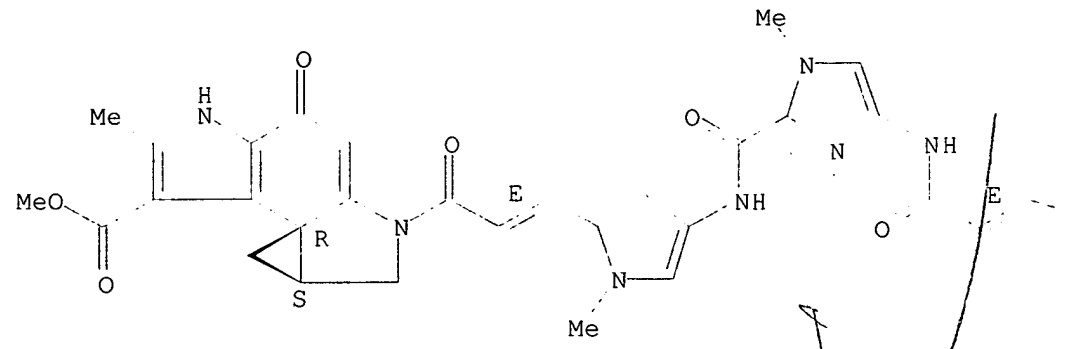
REFERENCE 1: 138:333279

REFERENCE 2: 135:371743

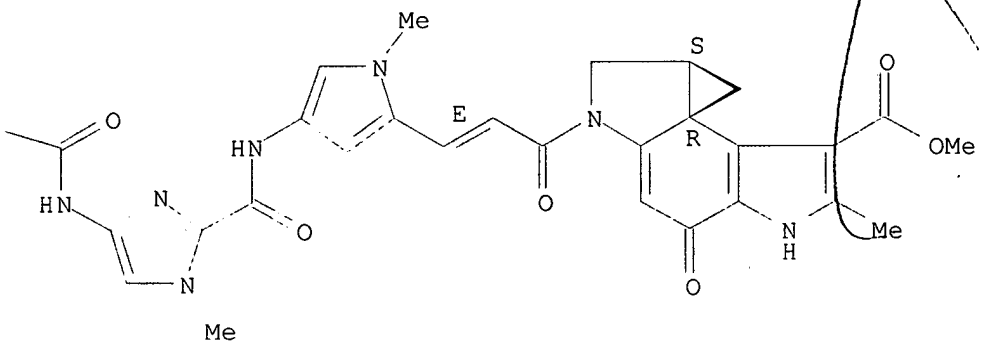
L11 ANSWER 12 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN
RN 373362-26-6 REGISTRY
CN Cyclopropa[c]pyrrolo[3,2-e]indole-7-carboxylic acid, 2,2'-[(1,4-dioxo-2-butene-1,4-diyl)bis[imino(1-methyl-1H-imidazole-4,2-diyl)carbonylimino(1-methyl-1H-pyrrole-4,2-diyl)[(2E)-1-oxo-2-propene-3,1-diyl]]]bis[1,2,4,5,8,8a-hexahydro-6-methyl-4-oxo-, dimethyl ester, (7bR,7'bR,8aS,8'aS)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C58 H54 N14 O12
SR CA
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



PAGE 1-B



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

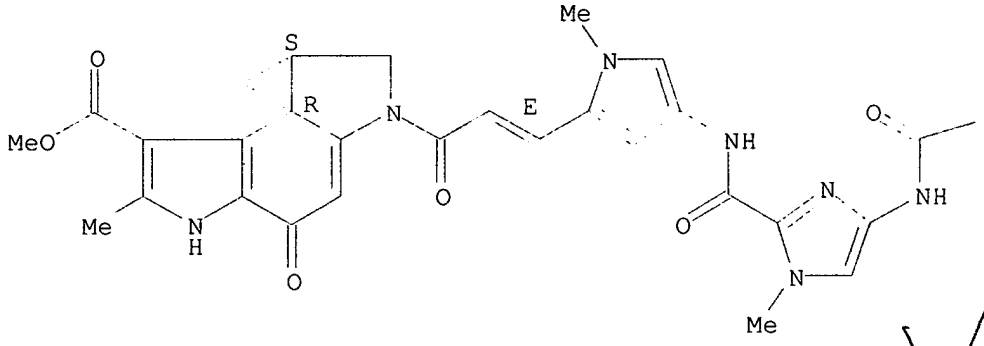
REFERENCE 1: 138:333279

REFERENCE 2: 135:371743

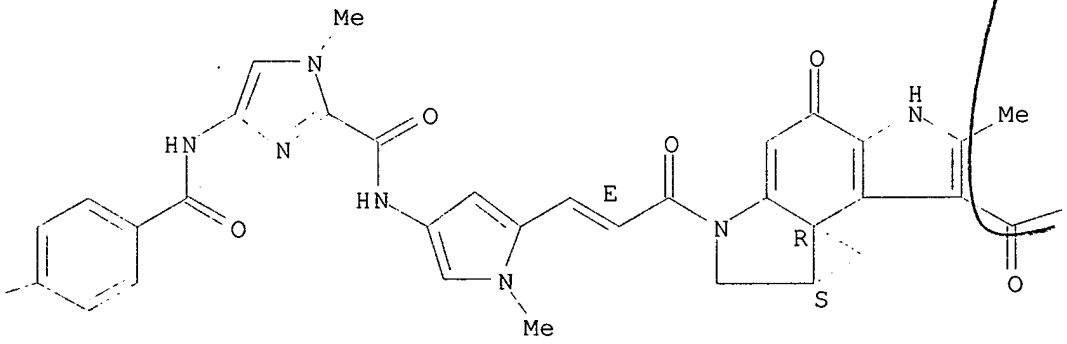
L11 ANSWER 13 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN
RN 373362-24-4 REGISTRY
CN Cyclopropa[c]pyrrolo[3,2-e]indole-7-carboxylic acid, 2,2'-[1,4-phenylenebis[carbonylimino(1-methyl-1H-imidazole-4,2-diyl)carbonylimino(1-methyl-1H-pyrrole-4,2-diyl)[(2E)-1-oxo-2-propene-3,1-diyl]]]bis[1,2,4,5,8,8a-hexahydro-6-methyl-4-oxo-, dimethyl ester, (7bR,7'bR,8aS,8'aS)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C62 H56 N14 O12
SR CA
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



PAGE 1-B



PAGE 1-C

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PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

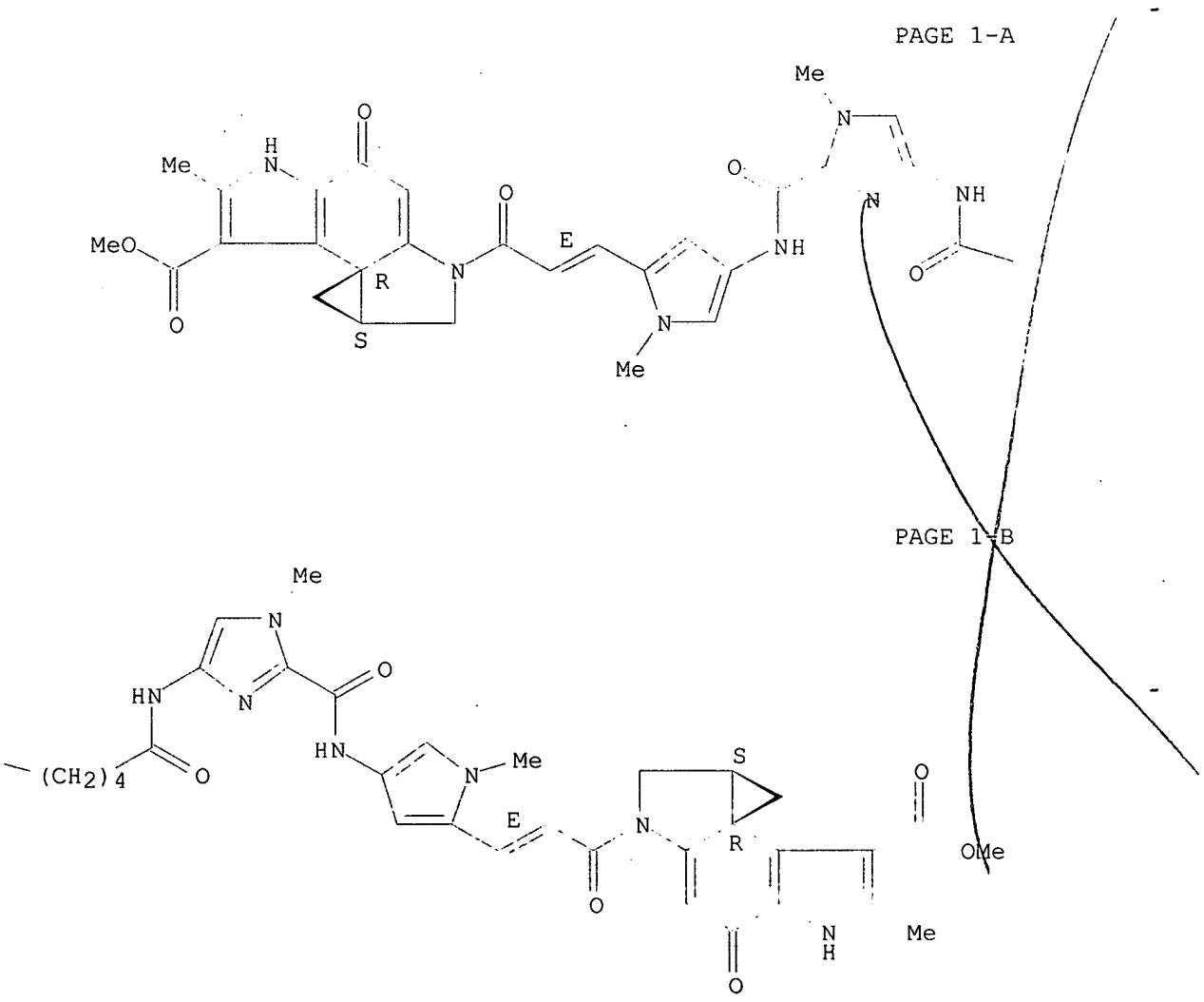
2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:333279

REFERENCE 2: 135:371743

L11 ANSWER 14 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN
RN 373362-22-2 REGISTRY
CN Cyclopropa[c]pyrrolo[3,2-e]indole-7-carboxylic acid, 2,2'-[(1,6-dioxo-1,6-hexanediyl)bis[imino(1-methyl-1H-imidazole-4,2-diyl)carbonylimino(1-methyl-1H-pyrrole-4,2-diyl)[(2E)-1-oxo-2-propene-3,1-diyl]]]bis[1,2,4,5,8,8a-hexahydro-6-methyl-4-oxo-, dimethyl ester, (7bR,7'bR,8aS,8'aS)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C60 H60 N14 O12
SR CA
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER

Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

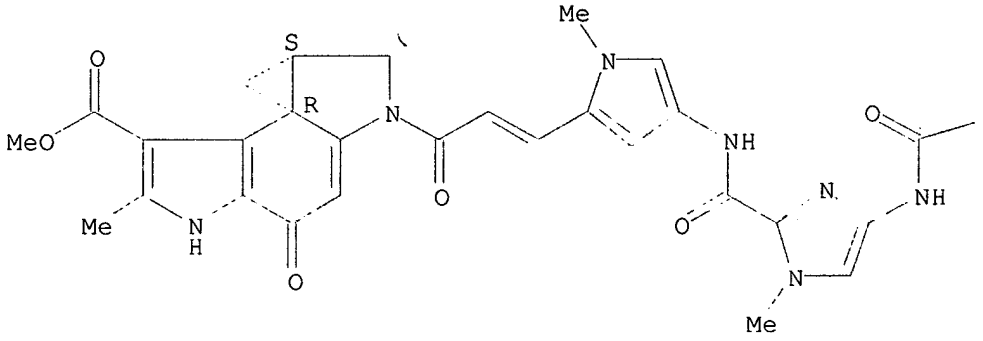
REFERENCE 1: 138:333279

REFERENCE 2: 135:371743

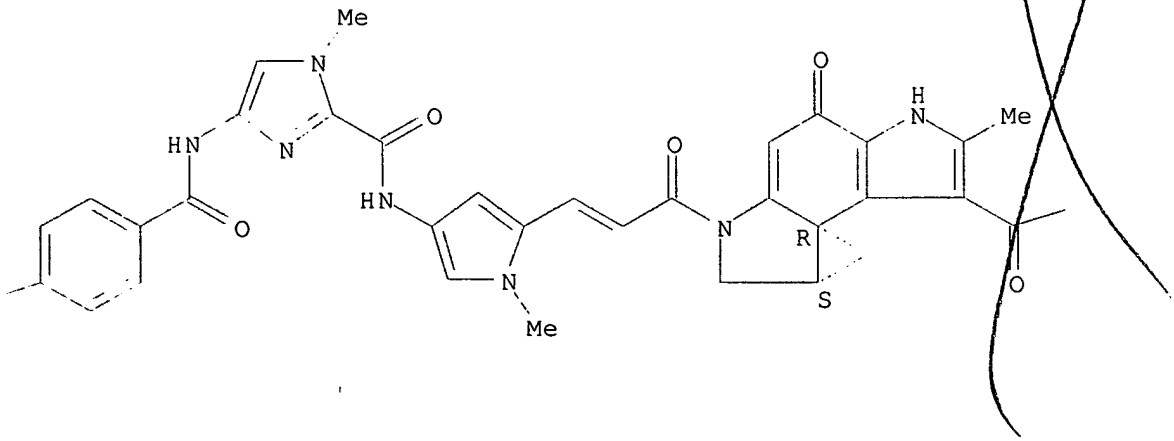
L11 ANSWER 15 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN
RN 349647-83-2 REGISTRY
CN Cyclopropa[c]pyrrolo[3,2-e]indole-7-carboxylic acid, 2,2'-[1,4-phenylenebis[carbonylimino(1-methyl-1H-imidazole-4,2-diyl)carbonylimino(1-methyl-1H-pyrrole-4,2-diyl)(1-oxo-2-propene-3,1-diyl)]]bis[1,2,4,5,8,8a-hexahydro-6-methyl-4-oxo-, dimethyl ester, (7bR,7'bR,8aS,8'aS)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C62 H56 N14 O12
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry unknown.

PAGE 1-A



PAGE 1-B



PAGE 1-C

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PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

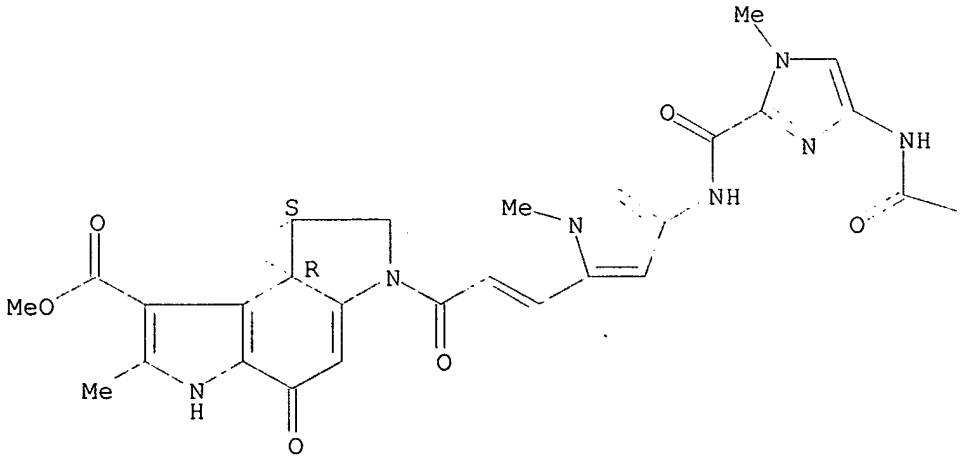
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 135:102536

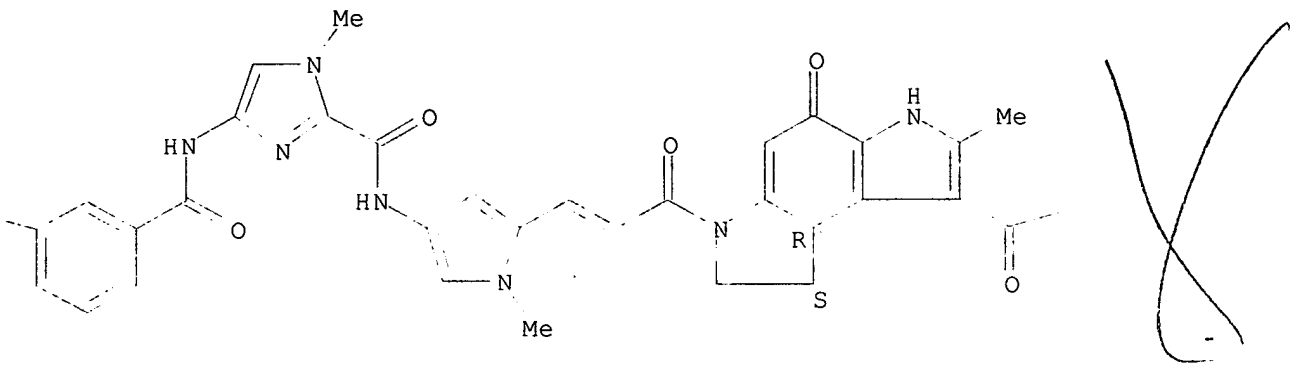
L11 ANSWER 16 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN
RN 349647-82-1 REGISTRY
CN Cyclopropa[c]pyrrolo[3,2-e]indole-7-carboxylic acid, 2,2'-[1,3-phenylenebis[carbonylimino(1-methyl-1H-imidazole-4,2-diyl)carbonylimino(1-methyl-1H-pyrrole-4,2-diyl)(1-oxo-2-propene-3,1-diyl)]]bis[1,2,4,5,8,8a-hexahydro-6-methyl-4-oxo-, dimethyl ester, (7bR,7'bR,8aS,8'aS)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C62 H56 N14 O12
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry unknown.

PAGE 1-A



PAGE 1-B



PAGE 1-C

OMe

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

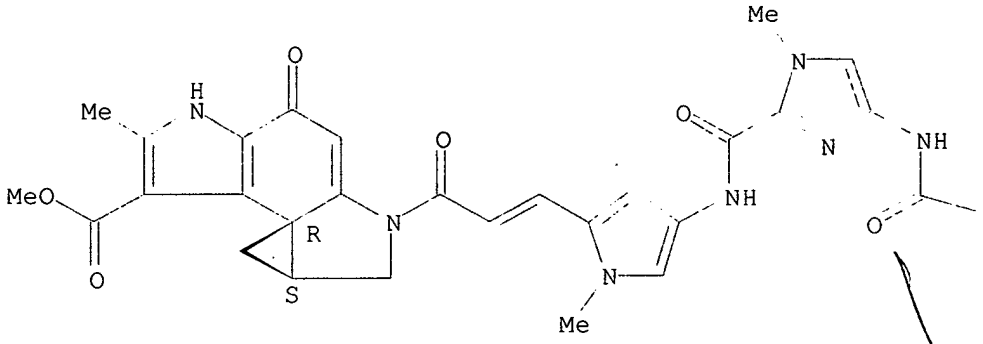
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 135:102536

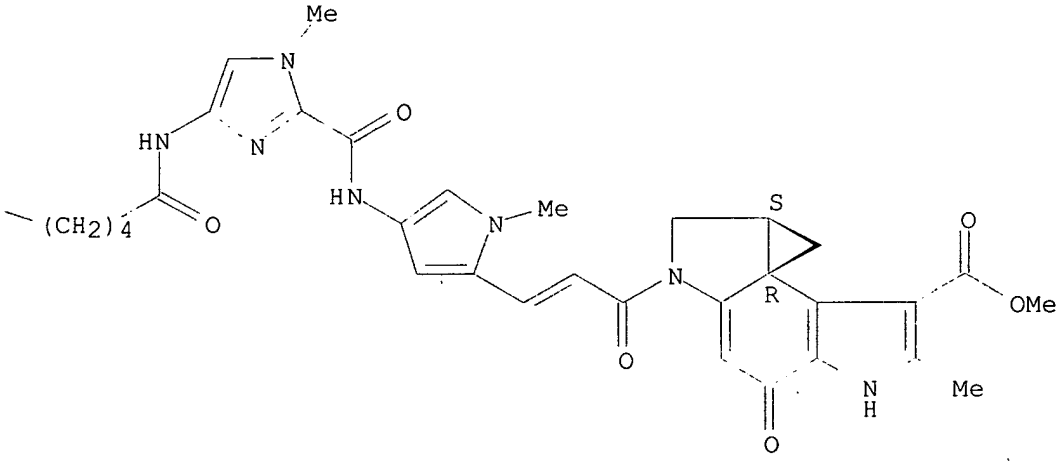
L11 ANSWER 17 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN
RN 349647-81-0 REGISTRY
CN Cyclopropa[c]pyrrolo[3,2-e]indole-7-carboxylic acid, 2,2'-[(1,6-dioxo-1,6-hexanediyl)bis[imino(1-methyl-1H-imidazole-4,2-diyl)carbonylimino(1-methyl-1H-pyrrole-4,2-diyl)(1-oxo-2-propene-3,1-diyl)]]bis[1,2,4,5,8,8a-hexahydro-6-methyl-4-oxo-, dimethyl ester, (7bR,7'bR,8aS,8'aS)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C60 H60 N14 O12
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry unknown.

PAGE 1-A



PAGE 1-B



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

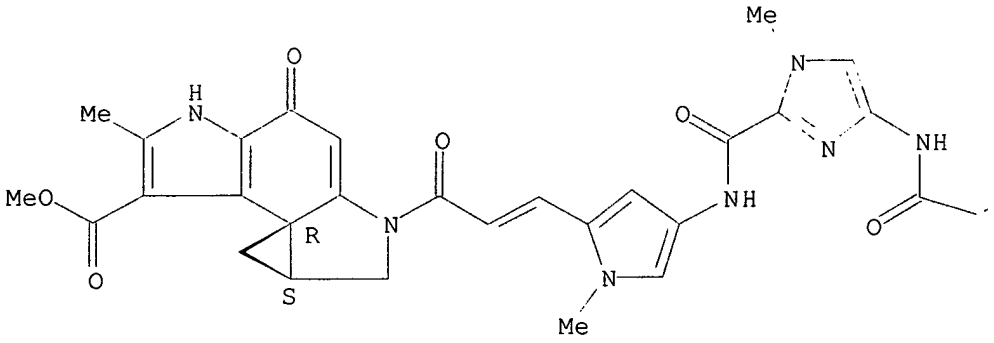
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 135:102536

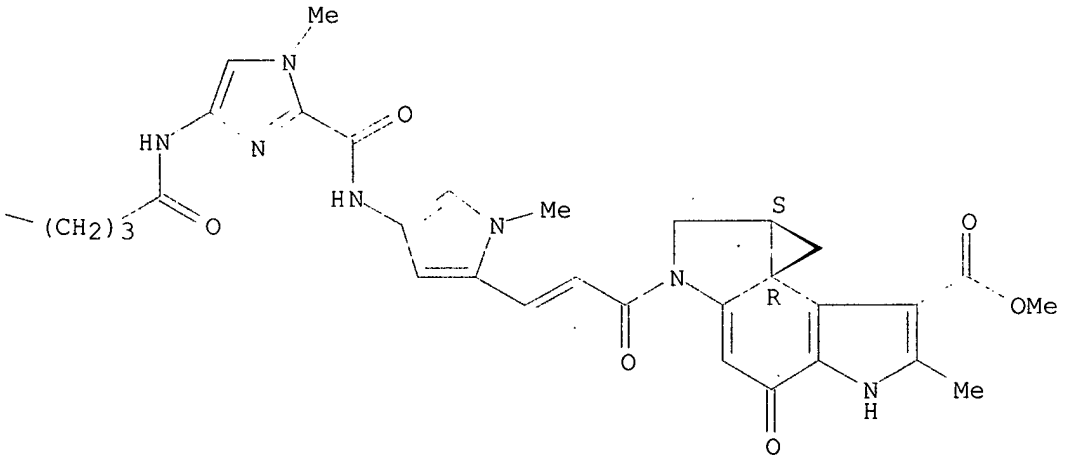
L11 ANSWER 18 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN
RN 349647-80-9 REGISTRY
CN Cyclopropa[c]pyrrolo[3,2-e]indole-7-carboxylic acid, 2,2'-[(1,5-dioxo-1,5-pentanediyl)bis[imino(1-methyl-1H-imidazole-4,2-diyl)carbonylimino(1-methyl-1H-pyrrole-4,2-diyl)(1-oxo-2-propene-3,1-diyl)]]bis[1,2,4,5,8,8a-hexahydro-6-methyl-4-oxo-, dimethyl ester, (7bR,7'bR,8aS,8'aS)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C59 H58 N14 O12
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry unknown.

PAGE 1-A



PAGE 1-B



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

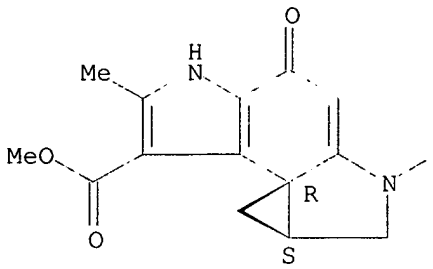
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 135:102536

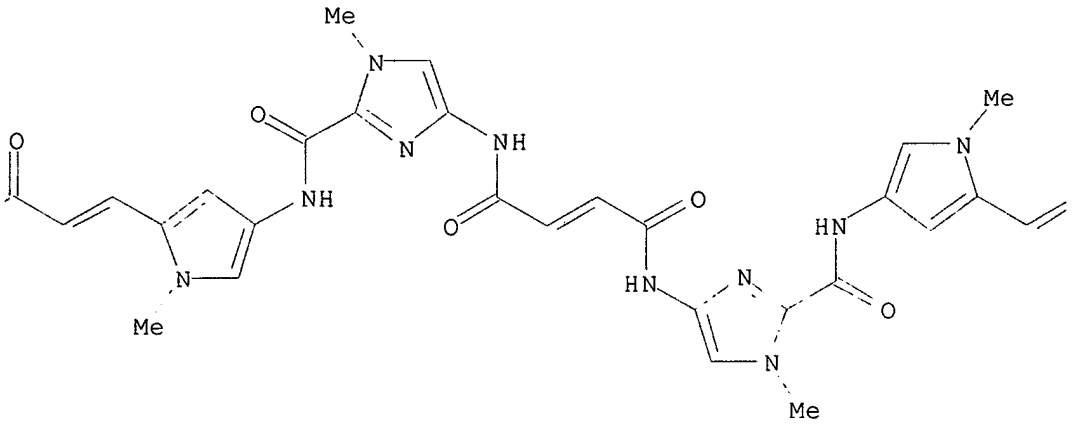
L11 ANSWER 19 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN
RN 349647-79-6 REGISTRY
CN Cyclopropa[c]pyrrolo[3,2-e]indole-7-carboxylic acid, 2,2'-[(1,4-dioxo-2-butene-1,4-diyl)bis[imino(1-methyl-1H-imidazole-4,2-diyl)carbonylimino(1-methyl-1H-pyrrole-4,2-diyl)(1-oxo-2-propene-3,1-diyl)]]bis[1,2,4,5,8,8a-hexahydro-6-methyl-4-oxo-, dimethyl ester, (7bR,7'bR,8aS,8'aS)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C58 H54 N14 O12
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry unknown.

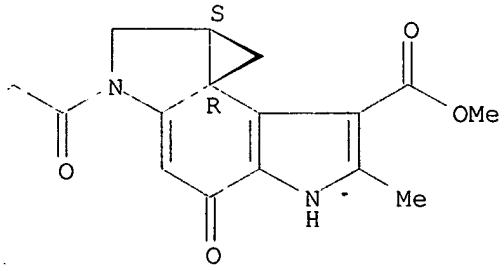
PAGE 1-A



PAGE 1-B



PAGE 1-C



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

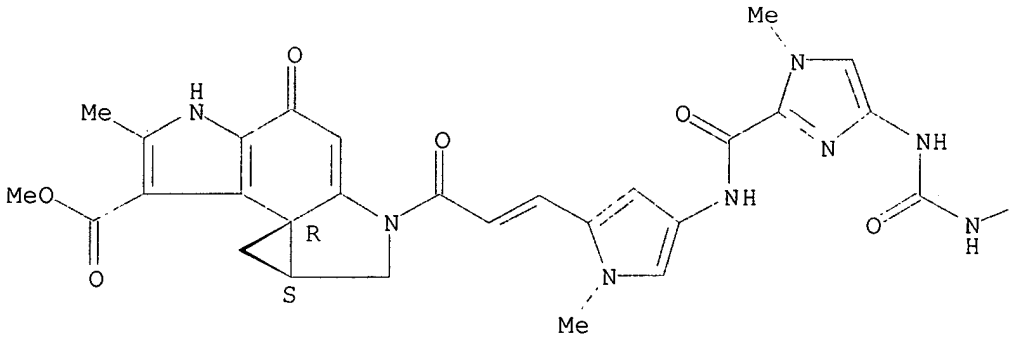
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 135:102536

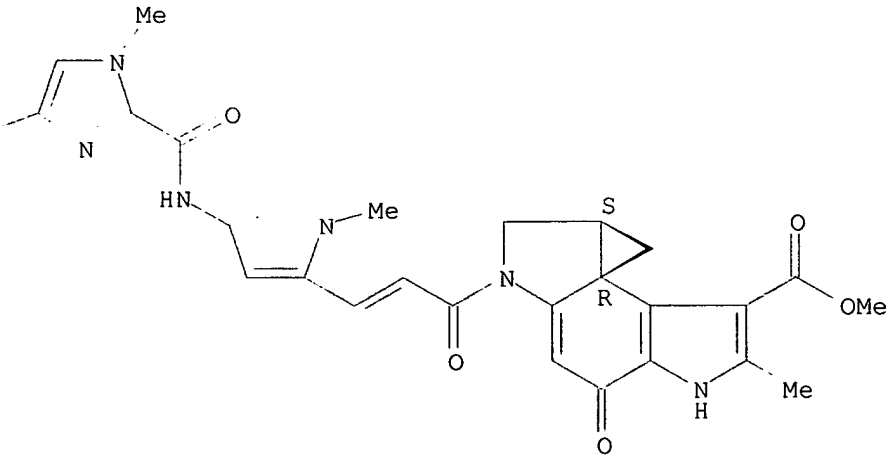
L11 ANSWER 20 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN
RN 349647-78-5 REGISTRY
CN Cyclopropa[c]pyrrolo[3,2-e]indole-7-carboxylic acid, 2,2'-[carbonylbis[imino(1-methyl-1H-imidazole-4,2-diyl)carbonylimino(1-methyl-1H-pyrrole-4,2-diyl)(1-oxo-2-propene-3,1-diyl)]]bis[1,2,4,5,8,8a-hexahydro-6-methyl-4-oxo-, dimethyl ester, (7bR,7'bR,8aS,8'aS)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C55 H52 N14 O11
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry unknown.

PAGE 1-A



PAGE 1-B



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

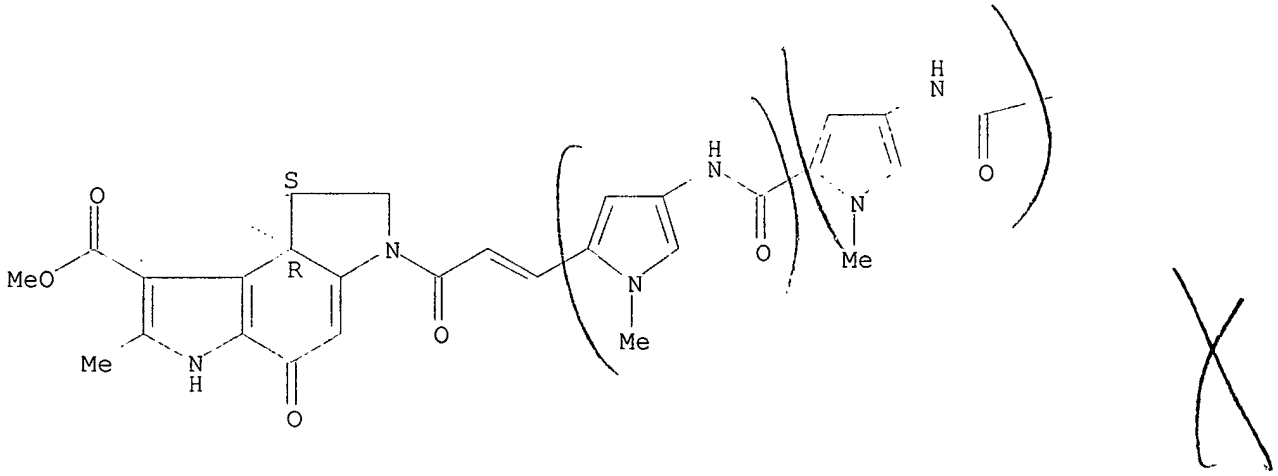
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 135:102536

L11 ANSWER 21 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN
RN 339984-92-8 REGISTRY
CN Cyclopropa[c]pyrrolo[3,2-e]indole-7-carboxylic acid, 2-[3-[4-[[[4-[[[4-(acetylamino)-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]-1-oxo-2-propenyl]-1,2,4,5,8,8a-hexahydro-6-methyl-4-oxo-, methyl ester, (7bR,8aS)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C36 H36 N8 O7
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.
Double bond geometry unknown.

PAGE 1-A



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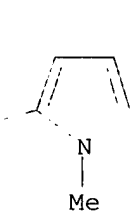


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

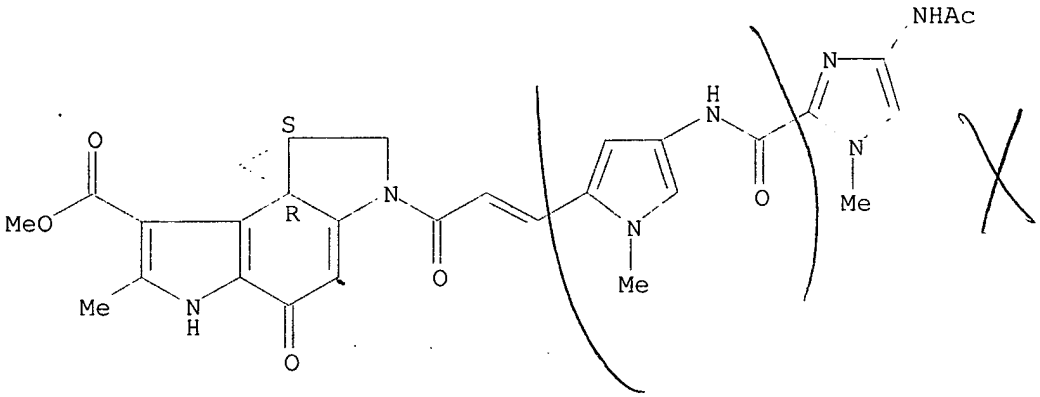
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 134:366795

L11 ANSWER 22 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN
RN 339984-91-7 REGISTRY
CN Cyclopropa[c]pyrrolo[3,2-e]indole-7-carboxylic acid, 2-[3-[4-[[[4-

(acetylamino)-1-methyl-1H-imidazol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]-1-oxo-2-propenyl]-1,2,4,5,8,8a-hexahydro-6-methyl-4-oxo-, methyl ester, (7bR,8aS)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C29 H29 N7 O6
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.
Double bond geometry unknown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

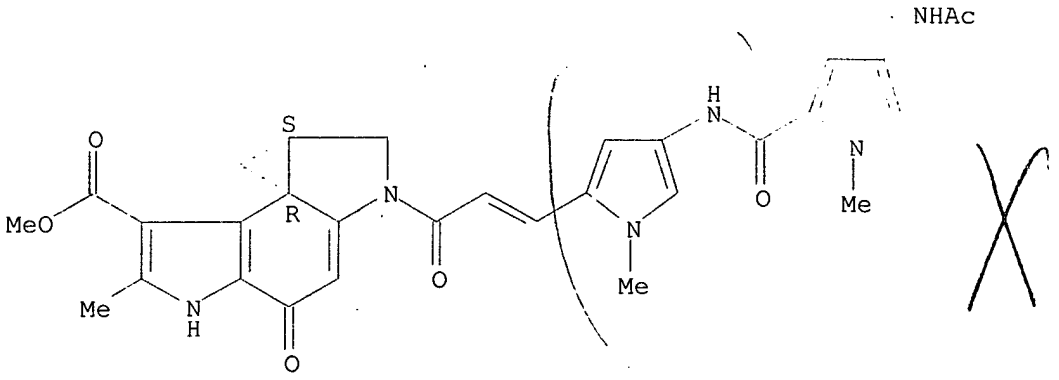
2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 139:345455

REFERENCE 2: 134:366795

L11 ANSWER 23 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN
RN 339984-88-2 REGISTRY
CN Cyclopropa[c]pyrrolo[3,2-e]indole-7-carboxylic acid, 2-[3-[4-[[[4-(acetylamino)-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]-1-oxo-2-propenyl]-1,2,4,5,8,8a-hexahydro-6-methyl-4-oxo-, methyl ester, (7bR,8aS)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C30 H30 N6 O6
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.
Double bond geometry unknown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

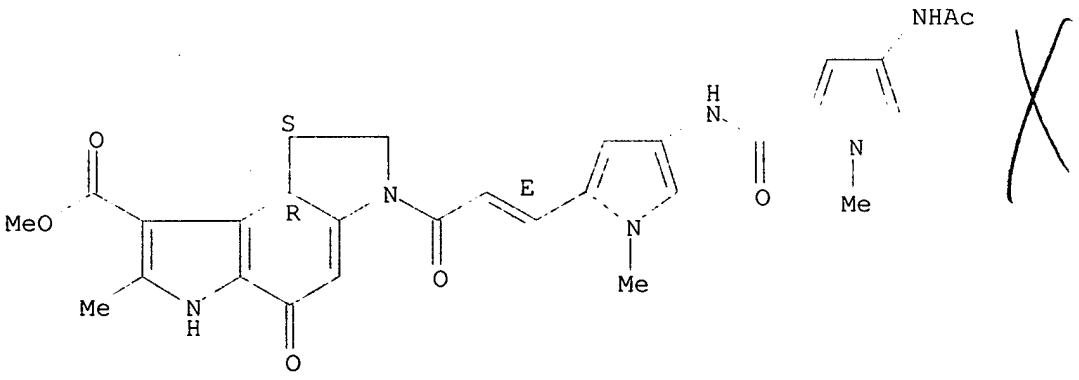
2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 139:345455

REFERENCE 2: 134:366795

L11 ANSWER 24 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN
RN 296794-38-2 REGISTRY
CN Cyclopropa[c]pyrrolo[3,2-e]indole-7-carboxylic acid, 2-[(2E)-3-[4-[[[4-(acetylamino)-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]-1-oxo-2-propenyl]-1,2,4,5,8,8a-hexahydro-6-methyl-4-oxo-, methyl ester, (7bR,8aS)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C30 H30 N6 O6
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.
Double bond geometry as shown.



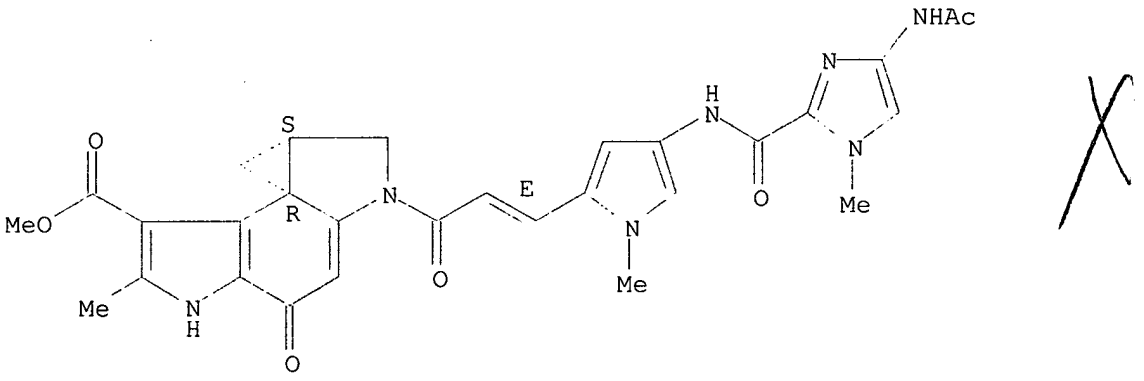
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 133:266852

L11 ANSWER 25 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN
RN 296794-37-1 REGISTRY
CN Cyclopropa[c]pyrrolo[3,2-e]indole-7-carboxylic acid, 2-[(2E)-3-[4-[[[4-(acetylamino)-1-methyl-1H-imidazol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]-1-oxo-2-propenyl]-1,2,4,5,8,8a-hexahydro-6-methyl-4-oxo-, methyl ester, (7bR,8aS)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C29 H29 N7 O6
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.
Double bond geometry as shown.



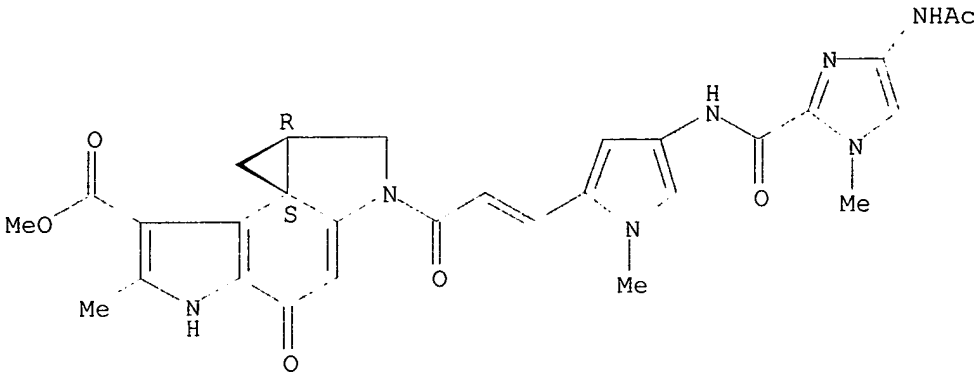
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 133:266852

L11 ANSWER 26 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN
RN 263710-69-6 REGISTRY
CN Cyclopropa[c]pyrrolo[3,2-e]indole-7-carboxylic acid, 2-[3-[4-[[[4-(acetylamino)-1-methyl-1H-imidazol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]-1-oxo-2-propenyl]-1,2,4,5,8,8a-hexahydro-6-methyl-4-oxo-, methyl ester, (7bS,8aR)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C29 H29 N7 O6
SR CA
LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry.
Double bond geometry unknown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:275556

L11 ANSWER 27 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN
RN 251999-81-2 REGISTRY
CN Cyclopropa[c]pyrrolo[3,2-e]indole-7-carboxylic acid, 2-[(2E)-3-[4-[[[4-[[[4-[[(1,1-dimethylethoxy)carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]-1-oxo-2-propenyl]-1,2,4,5,8,8a-hexahydro-6-methyl-4-oxo-, methyl ester, (7bR,8aS)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C39 H42 N8 O8
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.
Double bond geometry as shown.

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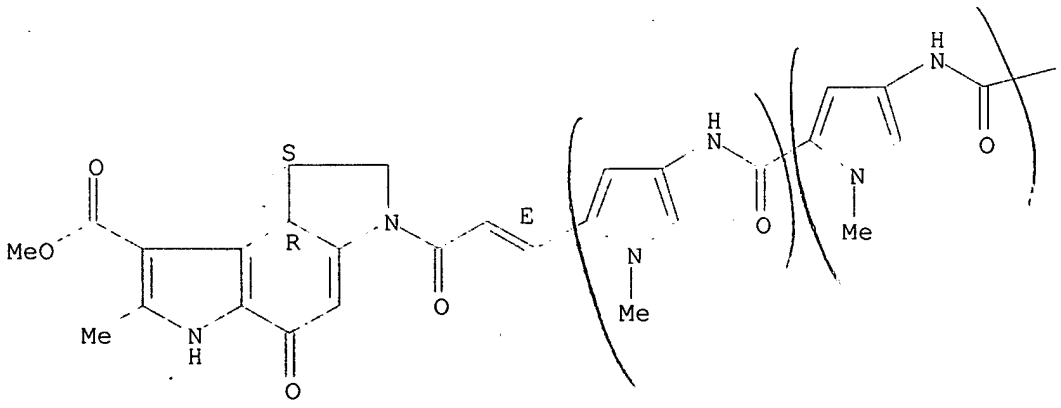

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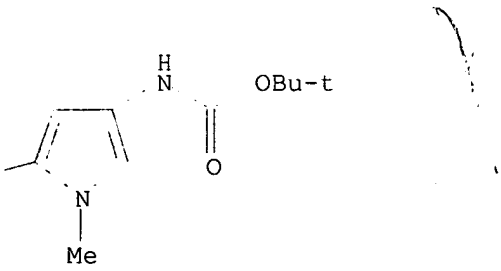


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

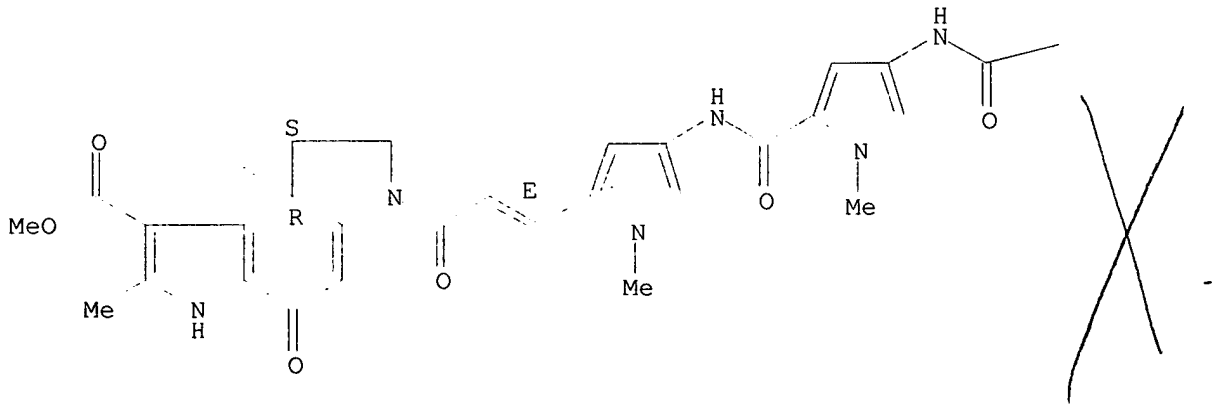
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:22791

L11 ANSWER 28 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN
RN 251999-80-1 REGISTRY
CN Cyclopropa[c]pyrrolo[3,2-e]indole-7-carboxylic acid, 2-[(2E)-3-[4-[[[4-[[(1,1-dimethylethoxy)carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]-1-oxo-2-propenyl]-1,2,4,5,8,8a-hexahydro-6-methyl-4-oxo-, methyl ester, (7bR,8aS)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C33 H36 N6 O7
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



PAGE 1-B

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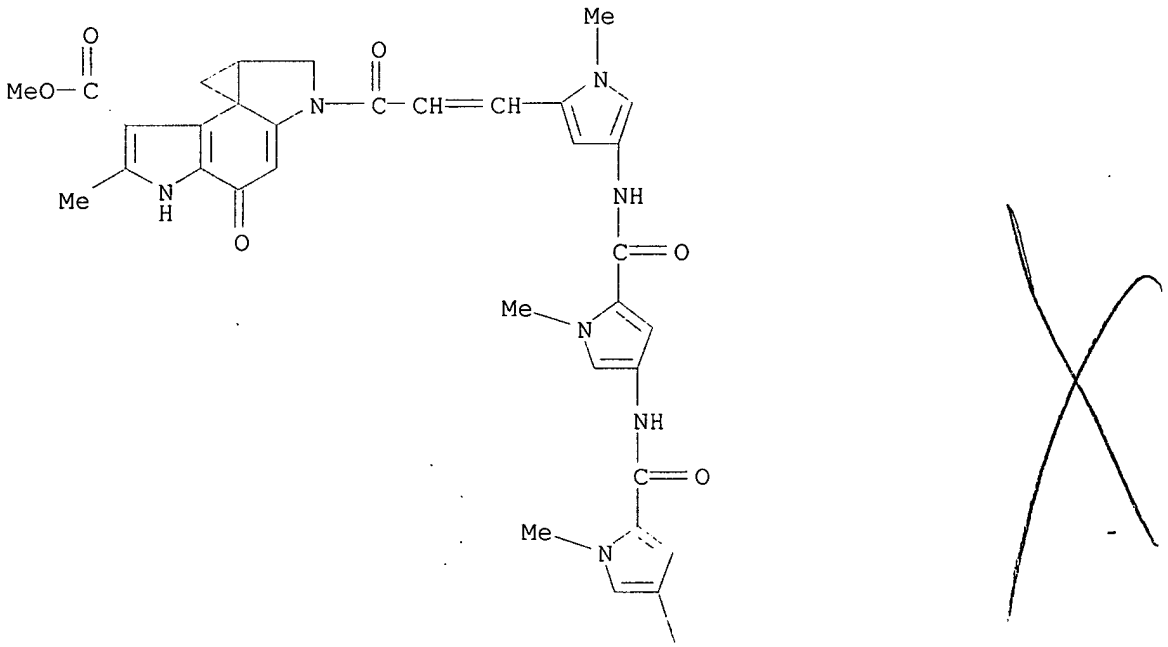
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

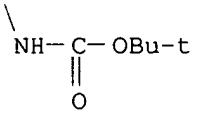
REFERENCE 1: 132:22791

L11 ANSWER 29 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN
RN 202419-15-6 REGISTRY
CN Cyclopropa[c]pyrrolo[3,2-e]indole-7-carboxylic acid, 2-[3-[4-[[[4-[[[4-[[(1,1-dimethylethoxy)carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]-1-oxo-2-propenyl]-1,2,4,5,8,8a-hexahydro-6-methyl-4-oxo-, methyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C39 H42 N8 O8
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

PAGE 1-A



PAGE 2-A



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

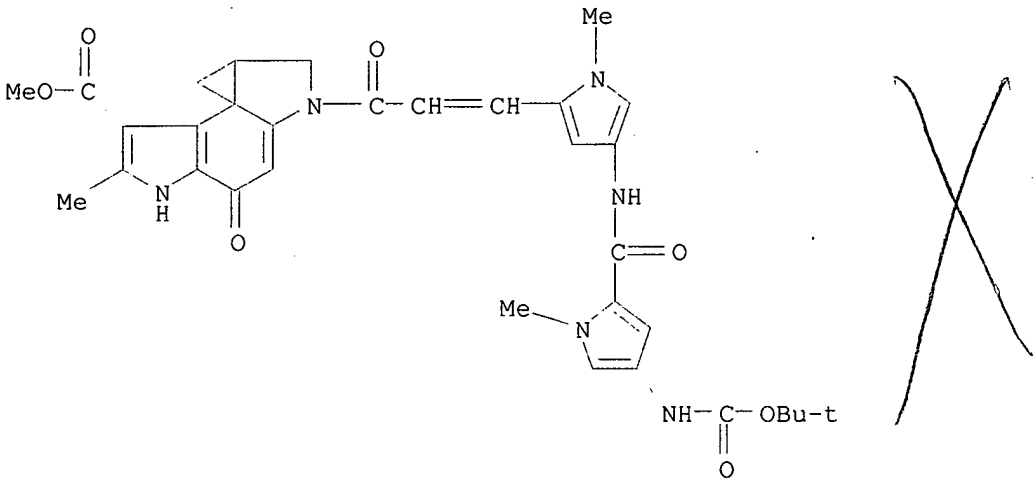
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 128:154100

L11 ANSWER 30 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN
RN 202419-12-3 REGISTRY
CN Cyclopropa[c]pyrrolo[3,2-e]indole-7-carboxylic acid, 2-[3-[4-[[[4-[[(1,1-

dimethylethoxy)carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]-1-oxo-2-propenyl]-1,2,4,5,8,8a-hexahydro-6-methyl-4-oxo-, methyl ester (9CI) (CA INDEX NAME)

FS 3D CONCORD
MF C33 H36 N6 O7
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 128:154100